A boundary integral method for the three-dimensional heat equation subject to specification of energy

W. T. Ang
Computational and Mathematical Sciences Group
Faculty of Information Technology
Universiti Malaysia Sarawak
94300 Kota Samarahan, Malaysia

A. B. Gumel
Department of Mathematics
University of Manitoba
Winnipeg, MB, Canada R3T2N2

Abstract

A boundary integral method is proposed for the numerical solution of the three-dimensional heat equation subject to specification of energy. A specific test problem is solved using the method.

Key words: boundary integral method, three-dimensional heat equation, Laplace transform, nonlocal condition.

This is the preprint of the article published in Journal of Computational and Applied Mathematics Vol 135 (2001) pp. 303-311.

1 INTRODUCTION

Consider solving the three-dimensional heat equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = \frac{\partial u}{\partial t} \tag{1}$$

for the unknown function $u(x, y, z, t)$ (the temperature) for $(x, y, z) \in V$ and $t \geq 0$, subject to the initial and boundary conditions

$$u(x, y, z, 0) = f(x, y, z) \text{ for } (x, y, z) \in V, \tag{2}$$

$$u(x, y, z, t) = g(x, y, z, t) \text{ for } (x, y, z) \in S_1 \text{ and } t \geq 0, \tag{3}$$

$$u(x, y, z, t) = h(x, y, z)q(t) \text{ for } (x, y, z) \in S_2 \text{ and } t \geq 0, \tag{4}$$

$$\frac{\partial}{\partial n}\left[u(x, y, z, t)\right] = k(x, y, z, t) \text{ for } (x, y, z) \in S_3 \text{ and } t \geq 0, \tag{5}$$

and the non-local (integral) condition

$$\iiint_V u(x, y, z, t)dxdydz = m(t) \text{ for } t \geq 0, \tag{6}$$

where V is a three-dimensional region bounded by a simple closed surface S, S_1, S_2 and S_3 are non-intersecting surfaces such that $S_1 \cup S_2 \cup S_3 = S$, f, g, h, k and m are suitably prescribed functions and q is an unknown function to be determined. Notice that $\partial u/\partial n = \mathbf{n} \cdot \nabla u$ where $\mathbf{n}$ is the unit normal vector on S pointing away from V. Notice that (6) specifies the total energy present in the region V at any time $t \geq 0$.

The problem defined by (1)-(6) arises in many important applications in heat transfer, control theory, thermoelasticity and medical science. To the best of the authors' knowledge, thus far, it has been solved only for cases where the unknown function u depends on one or at most two of the spatial variables x, y and z, see e.g. Cannon, Lin and Matheson [3]; Dehghan [4]; Gumel, Ang and Twizell [5]; Noye and Dehghan [6, 7]; Noye, Dehghan and van der Hoek [8]; Wang and Lin [12].

The present paper proposes a boundary integral method (BIM) for the numerical solution of the three-dimensional problem defined by (1)-(6) in the

Laplace transform (LT) space. The physical solution is recovered by using the Stehfest's algorithm [11] for the numerical inversion of the Laplace transformation. For the cases involving one- or two-dimensional physical spaces in the references cited above, the finite-difference methods are employed to solve the problem, usually for regions with special geometries such as a rectangular region. Thus, apart from extending the work to the three-dimensional physical space, the proposed BIM should provide a useful and interesting alternative to the finite-difference methods for solving this type of problems.

2 FORMULATION IN LT SPACE

Let us define the LT operator $\mathcal{L}$ on a function $r(x, y, z, t)$ $(t \geq 0)$ by

$$\mathcal{L}\{r(x, y, z, t); t \to p\} = \int_0^\infty r(x, y, z, t) \exp(-pt) dt \tag{7}$$

where p is the LT parameter. For our purpose here, we shall take p to be real and positive.

If we apply $\mathcal{L}$ on (1)-(6), the problem in the LT space is then to solve

$$\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2} - pU = -f(x, y, z) \tag{8}$$

for $U(x, y, z; p) = \mathcal{L}\{u(x, y, z, t); t \to p\}$ (for $(x, y, z) \in V$ and a suitably selected value of p) subject to

$$U(x, y, z; p) = G(x, y, z; p) \text{ for } (x, y, z) \in S_1, \tag{9}$$

$$U(x, y, z; p) = h(x, y, z)\Phi(p) \text{ for } (x, y, z) \in S_2, \tag{10}$$

$$\frac{\partial}{\partial n}\left[U(x, y, z; p)\right] = K(x, y, z; p) \text{ for } (x, y, z) \in S_3, \tag{11}$$

and

$$\iiint_V U(x, y, z; p) dx dy dz = M(p), \tag{12}$$

where

$$\begin{aligned} G(x,y,z;p) &= \mathcal{L}\{g(x,y,z,t);t\to p\},\\ \Phi(p) &= \mathcal{L}\{q(t);t\to p\},\\ K(x,y,z;p) &= \mathcal{L}\{k(x,y,z,t);t\to p\},\\ M(p) &= \mathcal{L}\{m(t);t\to p\}. \end{aligned} \tag{13}$$

Notice that $\Phi(p)$ is an unknown function to be determined.

Using (8) and the divergence theorem, we find that (12) can be rewritten as

$$\iint\limits_S \frac{\partial}{\partial n}\left[U(x,y,z;p)\right]\, ds = pM(p) - \iiint\limits_V f(x,y,z)dxdydz. \tag{14}$$

Notice that the right hand side of (14) is known and the left hand side containing an unknown function is expressed in terms of a surface integral.

To facilitate the task of solving (8)-(11) together with (14), we make the substitution

$$U(x,y,z;p) = U_{\text{part}}(x,y,z;p) + T(x,y,z;p), \tag{15}$$

where $U_{\text{part}}(x,y,z;p)$ is any particular solution of (8).

According to Atkinson [2], a particular solution of (8) is given by

$$U_{\text{part}}(x,y,z;p) = -\iiint\limits_R f(\xi,\eta,\psi)\Gamma(x,y,z;\xi,\eta,\psi;p)d\xi d\eta d\psi, \tag{16}$$

where $\Gamma(x,y,z;\xi,\eta,\psi;p)$ is given by (23) below (in Section 3) and R is a three-dimensional region which may be chosen to assume any specific geometry convenient for computing numerically the triple integral as long as $V \subseteq R$.

With the substitution in (15), (8)-(11) and (14) become:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} - pT = 0 \tag{17}$$

$$T(x,y,z;p) = G(x,y,z;p) - U_{\text{part}}(x,y,z;p) \text{ for } (x,y,z) \in S_1, \tag{18}$$

$$T(x,y,z;p) = h(x,y,z)\Phi(p) - U_{\text{part}}(x,y,z;p) \text{ for } (x,y,z) \in S_2, \tag{19}$$

$$\frac{\partial}{\partial n}\left[T(x,y,z;p)\right] = K(x,y,z;p) - \frac{\partial}{\partial n}\left[U_{\text{part}}(x,y,z;p)\right] \text{ for } (x,y,z) \in S_3, \tag{20}$$

$$\iint\limits_S \frac{\partial}{\partial n}\left[T(x,y,z;p)\right]\, ds = pM(p) - p\iiint\limits_V U_{\text{part}}(x,y,z;p)dxdydz. \tag{21}$$

3 BIM IN LT SPACE

If $\Phi(p)$ is known, the BIM for solving (17)-(20) is standard (Rizzo and Shippy [10]). As $\Phi(p)$ is unknown, the usual boundary integral procedure has to be *slightly* modified to take into consideration the extra equation (21).

For $(\xi,\eta,\psi) \in S \cup V$, the standard boundary integral solution of the homogeneous modified Helmholtz equation (17) is given by

$$\begin{aligned}\lambda(\xi,\eta,\psi)T(\xi,\eta,\psi;p) = \iint\limits_S \{&T(x,y,z;p)\frac{\partial}{\partial n}\left[\Gamma(x,y,z;\xi,\eta,\psi;p)\right] \\ &-\Gamma(x,y,z;\xi,\eta,\psi;p)\frac{\partial}{\partial n}\left[T(x,y,z;p)\right]\}ds,\end{aligned} \tag{22}$$

where $\lambda(\xi,\eta,\psi) = 1$ if $(\xi,\eta,\psi) \in V$ and $0 < \lambda(\xi,\eta,\psi) < 1$ if $(\xi,\eta,\psi) \in S$ and

$$\Gamma(x,y,z;\xi,\eta,\psi;p) = -\frac{1}{4\pi r}\exp(-r\sqrt{p}), \tag{23}$$

where $r = \sqrt{(x-\xi)^2 + (y-\eta)^2 + (z-\psi)^2}$.

The surface boundary S is discretized into N surface elements $S^{(1)}$, $S^{(2)}$,

..., $S^{(N-1)}$ and $S^{(N)}$. We make the following approximations:

$$S \approx S^{(1)} \cup S^{(2)} \cup ... \cup S^{(N-1)} \cup S^{(N)}, \tag{24}$$

$$T(x,y,z;p) \approx T^{(k)} \text{ for } (x,y,z) \in S^{(k)} \ (k = 1,2,...,N), \tag{25}$$

$$\frac{\partial}{\partial n}\left[T(x,y,z;p)\right] \approx W^{(k)} \text{ for } (x,y,z) \in S^{(k)} \ (k = 1,2,...,N), \tag{26}$$

where $T^{(k)}$ and $W^{(k)}$ $(k = 1,2,...,N)$ are constants to be determined.

With (24)-(26), by letting (ξ,η,ψ) be the midpoint of $S^{(i)}$ given by $(\xi^{(i)},\eta^{(i)},\psi^{(i)})$, (22) can be approximately rewritten as

$$\begin{aligned}\frac{1}{2}T^{(i)} = &\sum_{k=1}^{N}\left\{T^{(k)}\iint\limits_{S^{(k)}}\frac{\partial}{\partial n}\left[\Gamma(x,y,z;\xi^{(i)},\eta^{(i)},\psi^{(i)};p)\right]ds\right.\\ &\left.-W^{(k)}\iint\limits_{S^{(k)}}\Gamma(x,y,z;\xi^{(i)},\eta^{(i)},\psi^{(i)};p)ds\right\} \text{ for } i = 1,2,...,N.\end{aligned} \tag{27}$$

In (27), in taking $\lambda(\xi^{(i)},\eta^{(i)},\psi^{(i)}) = 1/2$, we assume that $(\xi^{(i)},\eta^{(i)},\psi^{(i)})$ lies on a smooth part of S.

Now if $\Phi(p)$ in (19) is given then from (18)-(20) either $T^{(k)}$ or $W^{(k)}$ (not both) is known over $S^{(k)}$. It follows that (27) constitutes a system of N linear algebraic equations in N unknowns. Since $\Phi(p)$ is not known, there are really $N+1$ unknowns. An additional equation is needed to complete the system of linear algebraic equations. This comes from (21) in the form:

$$\sum_{k=1}^{N}W^{(k)}A^{(k)} = pM(p) - p\iiint\limits_{V}U_{\text{part}}(x,y,z;p)dxdydz, \tag{28}$$

where $A^{(k)}$ is the area of the surface $S^{(k)}$.

Once $T^{(k)}$ and $W^{(k)}$ are determined, we can compute $T(x,y,z;p)$ at any

interior point (ξ, η, ψ) approximately via

$$T(\xi,\eta,\psi;p) \approx \sum_{k=1}^{N} \left\{ T^{(k)} \iint\limits_{S^{(k)}} \frac{\partial}{\partial n} \left[\Gamma(x,y,z;\xi,\eta,\psi;p)\right] ds \right.$$
$$\left. -W^{(k)} \iint\limits_{S^{(k)}} \Gamma(x,y,z;\xi,\eta,\psi;p) ds \right\}. \tag{29}$$

4 SOLUTION IN THE PHYSICAL SPACE

The physical solution $u(x,y,t)$ and $q(t)$ can be recovered approximately from $U(x,y;p)$ and $\Phi(p)$ by using a LT inversion technique. According to the Stehfest's algorithm [11] which is nowadays increasingly used in applied mechanics for the numerical inversion of LT (e.g. Ang [1]), we obtain

$$u(x,y,z,t) \approx \frac{\ln(2)}{t} \sum_{n=1}^{2P} c_n U\left(x,y,z;\frac{n\ln(2)}{t}\right),$$
$$q(t) \approx \frac{\ln(2)}{t} \sum_{n=1}^{2P} c_n \Phi\left(\frac{n\ln(2)}{t}\right), \tag{30}$$

where P is a positive integer and

$$c_n = (-1)^{n+P} \sum_{m=[(n+1)/2]}^{\min(n,P)} \frac{m^P (2m)!}{(P-m)!m!(m-1)!(n-m)!(2m-n)!}, \tag{31}$$

where $[r]$ denotes the integer part of the real number r. Note that each term in the LT inversion formula in (30) corresponds to one value of the LT transform parameter p, i.e. $p = n\ln(2)/t$.

As numerical techniques for inverting Laplace transform are highly susceptible to round-off errors, P cannot be selected to be as large as we like. On the other hand, choosing P to be too small may yield numerical results of lower accuracy. The optimum choice of P depends on the arithmetical precision of the computer (Stehfest [11]). Perhaps the best way to choose the optimum P is through testing the computer code of (30) on inverting known Laplace transforms of some elementary test functions.

5 A TEST PROBLEM

For a test problem, we take the region V to be $0 < x < 1$, $0 < y < 1$, $0 < z < 1$. The initial-boundary and nonlocal integral conditions are:

$$u(x,y,z,0) = \sin(\frac{\pi}{3}[x+y+z]) + xyz \text{ for } (x,y,z) \in V, \tag{32}$$

$$u(0,y,z,t) = q(t)\sin(\frac{\pi}{3}[y+z]) \text{ for } 0 < y < 1,\ 0 < z < 1,\ t \geq 0, \tag{33}$$

$$u(x,0,z,t) = \exp(-\frac{\pi^2 t}{3})\sin(\frac{\pi}{3}[x+z]) \text{ for } 0 < x < 1,\ 0 < z < 1,\ t \geq 0, \tag{34}$$

$$u(x,y,0,t) = \exp(-\frac{\pi^2 t}{3})\sin(\frac{\pi}{3}[x+y]) \text{ for } 0 < x < 1,\ 0 < y < 1,\ t \geq 0, \tag{35}$$

$$u(1,y,z,t) = \exp(-\frac{\pi^2 t}{3})\sin(\frac{\pi}{3}[1+y+z]) + yz \text{ for } 0 < y < 1,\ 0 < z < 1,\ t \geq 0, \tag{36}$$

$$u(x,1,z,t) = \exp(-\frac{\pi^2 t}{3})\sin(\frac{\pi}{3}[x+1+z]) + xz \text{ for } 0 < x < 1,\ 0 < z < 1,\ t \geq 0, \tag{37}$$

$$u(x,y,1,t) = \exp(-\frac{\pi^2 t}{3})\sin(\frac{\pi}{3}[x+y+1]) + xy \text{ for } 0 < x < 1,\ 0 < y < 1,\ t \geq 0, \tag{38}$$

$$\iiint_V u(x,y,z,t)dxdydz = \frac{27}{\pi^3}\exp(-\frac{\pi^2 t}{3}) + \frac{1}{8} \text{ for } t \geq 0. \tag{39}$$

The exact solution of the test problem is given by

$$u(x,y,z,t) = \exp(-\frac{\pi^2 t}{3})\sin(\frac{\pi}{3}[x+y+z]) + xyz \tag{40}$$

together with

$$q(t) = \exp(-\frac{\pi^2 t}{3}). \tag{41}$$

To implement the BIM, we take

$$\begin{aligned} &U_{\text{part}}(x, y, z; p) \\ &= -\iiint_V [\sin(\frac{\pi}{3}[\xi + \eta + \psi]) + \xi\eta\psi]\Gamma(x, y, z; \xi, \eta, \psi; p)d\xi d\eta d\psi. \end{aligned} \tag{42}$$

The triple integral has integrand with singularity of the type $1/r$ at $r = 0$, where r is the distance between (x, y, z) and (ξ, η, ψ). Numerical experiments indicate that integrals of this type can be evaluated with sufficient accuracy by repeated applications of the midpoint rule, i.e. using the quadrature

$$\int_0^1 \int_0^1 \int_0^1 g(\xi, \eta, \psi)d\xi d\eta d\psi \simeq h^3 \sum_{i=1}^{L} \sum_{j=1}^{L} \sum_{k=1}^{L} g(m_i, m_j, m_k), \tag{43}$$

where $h = 1/L$, L is a chosen positive even integer and $m_i = (2i-1)h/2$ (for $i = 1, 2, \cdots, L$). The triple integral in (28) which has well-behaved integrand is, however, evaluated numerically by using the trapezoidal rule, i.e.

$$\begin{aligned} &\int_0^1 \int_0^1 \int_0^1 U_{\text{part}}(x, y, z; p)dxdydz \\ &\simeq h^3 \sum_{i=1}^{L+1} \sum_{j=1}^{L+1} \sum_{k=1}^{L+1} b_i b_j b_k U_{\text{part}}(t_i, t_j, t_k; p), \end{aligned} \tag{44}$$

where h is as in (43), $b_1 = b_{L+1} = 1/2$ and $b_i = 1$ for $i = 2, 3, \cdots, L$ and $t_i = (i-1)h$ (for $i = 1, 2, \cdots, L+1$).

Each of the six faces of the cube which encloses the region V is discretized into L^2 square (boundary) elements of equal area h^2. Thus, the total number of boundary elements is given by $N = 6L^2$. The integrals in (27) and (29) over a boundary element are computed numerically by dividing the element equally into 4 smaller squares and applying the simple midpoint or the trapezoidal rule. [The midpoint rule is preferred if the integrand is singular

at some point on the surface element, i.e. if $i = k$ in (27).] The resulting linear algebraic equations are solved using the LU decomposition technique described in Press *et al.* [9].

Table 1. A comparison of the numerical and exact values of μ at selected time t.

t	$N = 216$	$N = 864$	Exact
0.10	0.6036	0.6589	0.7196
0.20	0.4517	0.4816	0.5179
0.30	0.3297	0.3470	0.3727
0.40	0.2381	0.2482	0.2682
0.50	0.1704	0.1764	0.1930

Table 2. A comparison of the numerical and exact values of $u(1/2, 1/2, 1/2, t)$ at selected time t.

t	$N = 216$	$N = 864$	Exact
0.10	0.8328	0.8364	0.8447
0.20	0.6299	0.6356	0.6429
0.30	0.4883	0.4921	0.4977
0.40	0.3868	0.3892	0.3932
0.50	0.3140	0.3154	0.3180

To obtain some numerical results, we use $L = 6$, i.e. 216 square boundary elements, each having sides of about 0.167 unit length ($h \simeq 0.167$), and 8 terms (i.e. $P = 4$) in the Laplace inversion formula (30) in order to compute $\mu(t)$ and $u(x, y, z, t)$. In Table 1, the numerical values of $\mu(t)$ together with the exact ones at selected time t are given. The numerical and the exact values of $u(x, y, z, t)$ are compared in Table 2 at the point $(1/2, 1/2, 1/2)$ and selected time t. The numerical results obtained using 216 elements can be regarded to be in reasonably good agreement with the exact solution, if we take into consideration the relatively coarse discretization of the boundary. The computation is repeated using 864 elements ($L = 12$ or $h \simeq 0.083$) and $P = 4$. The numerical results obtained are also presented in Tables 1 and 2. It is obvious that the calculation does yield better numerical results when the

discretization of the boundary is refined. The CPU time needed to complete the computation of both μ and u at a fixed given time t is about 25 seconds on a Pentium III 450 MHz (64 Mb SDRAM) desktop computer when 216 elements and $P = 4$ are used; it is about 770 seconds when 864 elements and $P = 4$ are used. (The proposed BIM is coded in double precision arithmetics using the Fortran 77 programming language.)

6 DISCUSSION

The problem of the three-dimensional heat equation subject to a nonlocal condition is considered. The nonlocal condition specifies the total energy in the system and is expressed in terms of a volume integral. The problem is reformulated in the LT space where the nonlocal condition is recast in a form in which the LT of the (unknown) normal derivative of the temperature is integrated on only the boundary of the solution domain. A simple BIM is then proposed for solving the problem in the LT space. The physical solution is retrieved by using a LT inversion technique. Volume integrals do appear in the proposed method but their integrands do not contain any unknown functions. Thus, as in a typical boundary-element method, the manipulation of the unknown data is restricted to only the boundary of the solution domain. Consequently, the number of unknowns involved is in general smaller than that which arises in other numerical techniques such as the finite-difference and the finite-element methods.

To obtain an indication of what is achievable by our simple BIM, we apply it to solve a specific test problem on a Pentium III desktop computer. The numerical results obtained clearly indicate that the proposed method works. Convergence of the numerical solution is observed when the calculation is refined by increasing the number of boundary elements.

The computational speed can be improved through parallel processing. The proposed method can be executed independently for different values of the LT parameter p. Thus, if the computation is carried out using a computer with $2P$ co-processors (one for each value of p), the CPU time needed can be

reduced by approximately a factor of $2P$. (Notice that the number of terms in the LT inversion formula is $2P$ and each term corresponds to one value of p. In solving the specific test problem, we use $P = 4$ and would therefore need to use 8 co-processors if all the terms in the inversion formula are to be computed simultaneously.)

Some factors affecting the computational speed of the proposed BIM are the efficiency of the solver for the linear algebraic equations and the numerical evaluations of the multiple integrals in (16) and (28). There are six integrations to carry out in the multiple integral in (28)! It appears that the CPU time required to execute the LU decomposition technique for solving the linear algebraic equations increases quite dramatically when the number of elements used is significantly increased. For example, in the specific test problem above, the CPU time used for the LU decomposition technique increases by over 100 times when the number of elements increases from 216 to 864, while the corresponding CPU time for the *entire* calculation (which includes boundary discretization, setting up the linear algebraic equations and solving them) increases by around 30 times only. These factors must be considered in any future studies if improvement in the computational speed is sought.

In the simple BIM proposed above, the LT of the temperature and its normal derivative are approximated as constant functions over a boundary element. The accuracy of the boundary element method can be improved by incorporating a higher order approximation over the boundary elements. With a higher order approximation, the implementation of the method on the computer may be expected to be more involved and complicated, however.

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