The Laplace transform boundary element methods for diffusion problems with periodic boundary conditions

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Abstract

The Laplace transform has been shown to be well-suited to the solution of diffusion problems and provides an alternative to the finite difference method. Such problems, parabolic in time, are transformed to elliptic problems in the space variables. Any suitable solver may be used in the space domain and a numerical inversion of the transform is then performed. For parabolic problems the Stehfest numerical method has been shown to be accurate, robust and easy to implement. The boundary element method has been used by a variety of authors to solve the resulting elliptic problem. The initial conditions lead to a non-homogenous Helmholtz-type problem which may be solved using the dual reciprocity method. Time-dependent boundary conditions are, in principle, easily implemented. However, problems can occur if the conditions are not monotonic in time. The authors have already considered problems with a discontinuity in the boundary condition and have shown that the Laplace transform can be used to find the solution up to the discontinuity and then, using the computed solution as a new initial condition, to proceed past the continuity. Similarly, for boundary conditions with period $2T$, the Laplace transform is used in time intervals of length $\frac{1}{2}T$, where the boundary condition is monotonic, and the computed solution at time $\frac{1}{2}T$ is used to move on to the next monotonic phase.
Keywords: boundary element method, Laplace transform, periodic boundary condition, dual reciprocity method.

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1 Introduction

In the numerical solution of parabolic problems the most common approach to the solution is to use a finite difference time-stepping process. At each time step a solution of an elliptic problem is required and the boundary element method provides a suitable approach. A variety of schemes has been produced, Honnor *et al.* [1] describe a generalised approach in which all the 'usual' methods may be recovered as special cases. A problem that occurs with time-stepping processes is that there may be severe stability restrictions. An alternative approach is to use the Laplace transform in time. Rizzo and Shippey [2] first used the Laplace transform in conjunction with the boundary integral equation method using an inversion process in terms of a Prony series of negative exponentials in time. Stefhest's method, which is much simpler to apply, was first used by Moridis and Reddell [3]. Provided that the boundary conditions are monotonic in time, the solution is developed directly at one specific time value without the necessity of intermediate values. If the solution is required at one particular time only then the current approach is particularly useful since just one application of the Laplace transform boundary element method is needed giving a significant saving in computational effort. In sections we shall show that even if the boundary conditions are not monotonic then a piecewise application still yields a significant saving in computational effort. If the time history is required then the solution may be developed at any set specified times. Once a numerical solution of the elliptic problem has been effected then Stehfest's method [4, 5] provides a numerical Laplace transform inversion which is simple to use, provides accurate results and is recommended by Davies and Martin [6] in their study of a variety of numerical Laplace transform inversion methods.

2 The Laplace transform method for diffusion problems

Consider the initial boundary-value problem defined in the two-dimensional region Ω bounded by the closed curve $\Gamma = \Gamma_1 + \Gamma_2$

$$\nabla^2 u = \frac{1}{\alpha}\frac{\partial u}{\partial t} \quad \text{in } D \tag{1}$$

subject to the boundary conditions

$$u = u_1(s,t) \text{ on } \Gamma_1 \tag{2}$$

$$q \equiv \frac{\partial u}{\partial n} = q_2(s,t) \text{ on } \Gamma_2 \tag{3}$$

and the initial condition

$$u(x,y,0) = u_0(x,y)\,. \tag{4}$$

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We now define the Laplace transform in time by

$$\bar{u}(x;\lambda)=\int_0^\infty u(x,t)e^{-\lambda t}dt \tag{5}$$

so that the initial boundary-value problem (1), (2), (3) and (4) becomes

$$\nabla^2\bar{u}=\frac{1}{\alpha}\left(\lambda\bar{u}-u_0\right) \text{ in } \Omega \tag{6}$$

subject to

$$\bar{u}=\bar{u}_1(s;\lambda) \text{ on } \Gamma_1 \tag{7}$$

$$\bar{q}=\bar{q}_2(s;\lambda) \text{ on } \Gamma_2. \tag{8}$$

In the case $u_0 \equiv 0$ equation (6) becomes homogeneous. Similarly if u_0 is harmonic in Ω we can make a change in the dependent variable to obtain a homogeneous equation. In both cases the resulting elliptic equation (6) may be solved by a variety of methods, *e.g.* Davies *et al.* [7] use finite elements, finite differences, fundamental solutions and boundary elements. We shall restrict ourselves to the boundary element method for which a suitable fundamental solution is

$$\bar{u}^*=\frac{1}{2\pi}K_0\left(\sqrt{\frac{\lambda}{\alpha}}R\right) \tag{9}$$

where R is the distance from the source point to the field point (x,y). K_i is the modified Bessel function of the second kind. This has been applied successfully by a variety of authors [8, 9]. In her investigation of the suitability of the Laplace transform for diffusion-type problems, Crann [10] showed that difficulties can occur with the numerical inversion if the functions involved are not monotonic in the time variable. In particular she considers a problem with a shock discontinuity in the boundary condition [11, 13] showing that the difficulty is associated with the recovery of the discontinuity since this is smoothed out by the Laplace transform process. However, if the solution is found up to the discontinuity then this solution can be used as an initial condition for the post-shock solution. For diffusion problems Williams [12] shows that oscillatory solutions exist only if the boundary conditions or an internal source functions are oscillatory. Crann and Davies [13] have shown, using finite differences for the elliptic problem, that such solutions can be recovered if the Laplace transform is applied in a piecewise manner, tracking oscillations between successive regions of monotonicity. We shall use the same approach using the boundary element method for the elliptic problem. However, the resulting equation (6) is no longer homogeneous and we must use a suitable approach to handle the non-homogeneity. The dual reciprocity method [14]

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allows us to do this and at the same time use the simpler Laplacian fundamental solution

$$\bar{u}^* = -\frac{1}{2\pi}\ln(R) \qquad (10)$$

3 The dual reciprocity method

It is very simple to add a reaction term, $F(x,y,t)$, in equation (1) which leads to an extra term of the form $\bar{F}(x,y;\lambda)$ in equation (6) which, using the fundamental solution (10), we can write as

$$\nabla^2\bar{u} = b(x,y,\bar{u};\lambda) \text{ in } \Omega \qquad (11)$$

subject to the same boundary conditions (7) and (8).

By using the fundamental solution (10) and Green's theorem, equation (11) can be written in the integral form

$$c_i\bar{u}_i + \int_\Gamma \bar{q}^*\bar{u}_i d\Gamma - \int_\Gamma \bar{u}^*\bar{q}_i d\Gamma + \int_\Omega b_i\bar{u}^* d\Omega = 0 \qquad (12)$$

In the dual reciprocity method we approximate the right-hand side of equation (11) in terms of a linear combination of radial basis functions, $f_j(R)$, in the form

$$b_i = \sum_{j=1}^{M}\alpha_j f_j(R_i) \qquad (13)$$

where b_i is the value of the function b at node i. The collocation is performed at the $M = N + L$ nodes, where N and L are the numbers of boundary and internal nodes respectively.

The functions $f_j(R)$ are chosen so that we can find a particular solution, $\hat{\bar{u}}$, with the property $\nabla^2\hat{\bar{u}}_j = f_j$.

Using these values in equation (12) and using Green's theorem we obtain the boundary integral form

$$c_i\bar{u}_i + \int_\Gamma \bar{q}^*\bar{u}_i d\Gamma - \int_\Gamma \bar{u}^*\bar{q}_i d\Gamma = \sum_{j=1}^{N}\left\{\alpha_j\left(c_i\hat{\bar{u}}_{ij} + \int_\Gamma \bar{q}^*\hat{\bar{u}}_j d\Gamma - \int_\Gamma \bar{u}^*\hat{\bar{q}}_j d\Gamma\right)\right. \qquad (14)$$

Internal values are given by

$$c_i\bar{u}_i = -\int_\Gamma \bar{q}^*\bar{u}_i d\Gamma + \int_\Gamma \bar{u}^*\bar{q}_i d\Gamma + \sum_{j=1}^{L}\left\{\alpha_j\left(c_i\hat{\bar{u}}_{ij} + \int_\Gamma \bar{q}^*\hat{\bar{u}}_j d\Gamma - \int_\Gamma \bar{u}^*\hat{\bar{q}}_j d\Gamma\right)\right. \qquad (15)$$

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Combining equations (14) and (15) and collocating at the M points yields the overall set of equations

$$\mathbf{H\bar{U}} - \mathbf{G\bar{Q}} = \left[\mathbf{H\hat{\bar{U}}} - \mathbf{G\hat{\bar{Q}}} \right] \mathbf{F}^{-1}\mathbf{b} \tag{16}$$

where the matrix $\mathbf{F}$ is the collocation matrix from equation (13) written in the form $\mathbf{b} = \mathbf{F}\alpha$.

The solution of equation (16) yields the approximate transforms $\bar{\mathbf{U}}$ and $\bar{\mathbf{Q}}$ which may then be inverted to obtain the approximate solutions $\mathbf{U}$ and $\mathbf{Q}$.

To implement the Stehfest we proceed as follows:
Choose a specific time value, τ, at which we seek the solution and define a discrete set of transform parameters given by

$$\left\{ \lambda_j = j\frac{\ln 2}{\tau} : \quad j = 1, 2, ..., m;\ m \text{ even} \right\}. \tag{17}$$

The boundary element method is applied to equation (13) for each λ_j to obtain a set of approximate boundary values

$$\bar{U}_{ij},\ i = 1, ..., N; \quad j = 1, ..., m$$

and a set of approximate internal values

$$\bar{U}^I_{kj}, \quad k = 1, ..., L; \quad j = 1, ..., m\ .$$

The inverse transforms are then given as follows:

$$U_r = \frac{\ln 2}{\tau} \sum_{j=1}^{M} w_j \bar{U}_{rj} \tag{18}$$

and

$$U^I_r = \frac{\ln 2}{\tau} \sum_{j=1}^{M} w_j \bar{U}^I_{rj} \tag{19}$$

where $r = 1...N$ for boundary points and $r = 1...L$ for internal points.

The weights, w_j, are given by Stehfest [4, 5] as

$$w_j = (-1)^{\frac{m}{2}+j} \sum_{k=\frac{1}{2}[1+j]}^{\min\left(j, \frac{m}{2}\right)} \frac{k^{\frac{m}{2}} (2k)!}{\left(\frac{m}{2} - k\right)! k! (k-1)! (j-k)! (2k-j)!}\ . \tag{20}$$

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4 Periodic boundary conditions

Suppose that the time-dependent boundary conditions (2) and (3) are periodic, *e.g.* $u_1(s,t+T)=u_1(s,t)$ and $q_2(s,t+T)=q_2(s,t)$, we apply the Laplace transform piecewise in time and seek solutions, $u^{(i)}(x,y)$ in the intervals $t_i \le t \le t_i + \frac{1}{4}T$, $i=1,2,...$ as follows:

Solve

$$\nabla^2 u^{(i)} = \frac{1}{\alpha}\frac{\partial u^{(i)}}{\partial t} + F(x,y,t) \quad \text{in } D,\ t_i \le t \le t_i + \tfrac{1}{4}T \tag{21}$$

subject to the boundary conditions

$$u^{(i)} = u_1(s,t) \text{ on } \Gamma_1 \text{ and } q^{(i)} = q_2(s,t) \text{ on } \Gamma_2 \tag{22}$$

and the initial condition

$$u^{(i)}(x,y,0) = u^{(i-1)}(x,y,t_i + \tfrac{1}{4}T) \tag{23}$$

We effect the Laplace transform solution by making the change of variable $t = \tau + \frac{1}{4}T$ and so the problem is now defined in $0 \le \tau \le \frac{1}{4}T$.

5 Results

The two examples in this section are defined in the unit square $\{(x,y): 0<x<1,\ 0<y<1\}$ using $N=32$ boundary points and $L=9$ internal points. Also, in the dual reciprocity method, we use thin plate splines, $R^2 \ln R$, augmented with a linear term $a+bx+cy$, for the basis functions in equation (13). For the numerical Laplace transform we use the Stehfest parameter value $m=8$.

Example 1

In this problem $\alpha=1$ and the non-homogeneous term is given by $F(x,y,t) = -2x\sin t - xy(1-y)\cos t$.

The boundary conditions are given by
$u=1$ on $x=0,\ y=0$ and $y=1$; $u=1+y(1-y)\sin t$ on $x=1$
and the initial condition is
$u(x,y,0)=1$.

We see that the boundary conditions have period 2π.

The analytic solution is given by $u(x,y,t)=1+xy(1-y)\sin t$.

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In Figure 1 we show the time development of the approximate solution, $U_r(t)$, and the analytic solution, $u(x,y,t)$, at the point $(0.25, 0.25)$ plotted over the interval $0 \le t \le \frac{5}{2}\pi$.

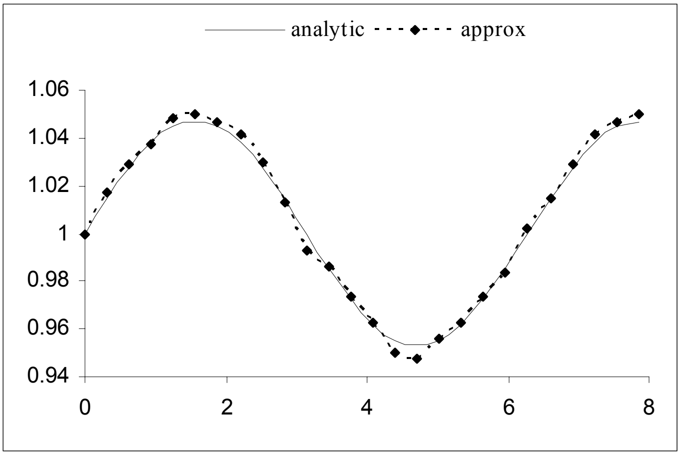

Figure 1: Time development of the solution at $(0.25, 0.25)$ for $0 \le t \le \frac{5}{2}\pi$.

We notice that, in the first period, the approximate solution tracks the analytic solution very well; the largest errors are found for values of t close to $t = \frac{1}{2}\pi$ and $t = \frac{3}{2}\pi$ and these errors are less than 1%. We also notice that the approximate solution is clearly exhibiting the correct periodic behaviour, tracking the analytic solution very well in the second period. Clearly, we can now predict approximate future values using the periodicity relationship $U_r(t) = U_r(t - 2n\pi)$ when $2n\pi \le t \le (2n+1)\pi$.

The solution in this example does not exhibit a transient part, the initial and boundary conditions are such that the system is configured in the steady-state at time $t = 0$. In the following example we consider a problem whose solution exhibits a transient term.

Example 2

In this problem $\alpha = 0.2$ and the non-homogeneous term is given by $F(x,y,t) = -\frac{\pi}{\alpha} x \cos(\pi t)$.

The boundary conditions are given by
$u = 0$ on $x = 0$; $q = 0$ on $y = 0$ and $y = 1$; $u = \sin(\pi t)$ on $x = 1$
and the initial condition is

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$u(x, y, 0) = \sin(\pi x)$.

We see that the boundary conditions have period 2.

The analytic solution is given by $u(x, y, t) = \exp(-\alpha\pi^2 t)\sin(\pi x) + x\sin(\pi t)$.

In Figure 2 we show the time development of the approximate solution, $U_r(t)$, and the analytic solution, $u(x, y, t)$, at the point $(0.25, 0.25)$ plotted over $3\frac{1}{2}$ periods, *i.e.* over the interval $0 \le t \le 7$.

We notice that the solution tracks the transient part very well and is in good general agreement with the steady-state term. The numerical solution suggests that the transient term has disappeared by $t = 3$. In fact in the analytic solution the transient term has a magnitude of the order of 0.002 at $t = 3$ *i.e.* smaller than the steady-state term by a factor of about 100. The largest errors are at the points corresponding to maximum values of $|u|$ and these predict the steady-state amplitude to have an error of the order of approximately 10%.

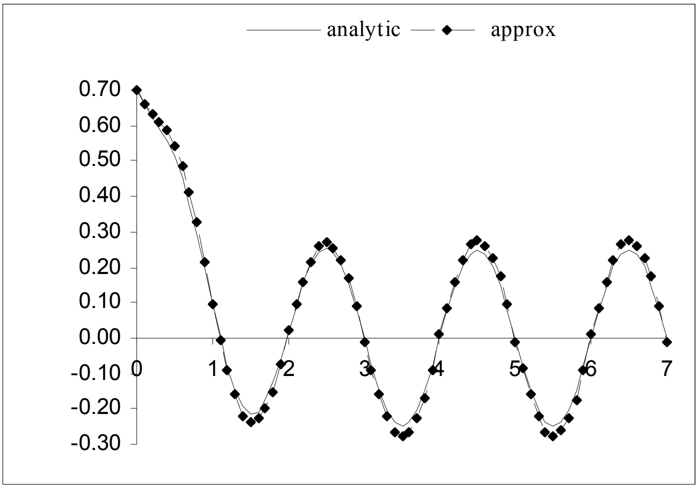

Figure 2: Time development of the solution at $(0.25, 0.25)$ for $0 \le t \le 7$.

6 Conclusions

The numerical Laplace transform method in time together with the boundary element method in space offers an excellent approach to the solution process for diffusion-type problems. Stehfest's method provides a numerical inversion process which is both accurate and easy to implement and does not suffer from potential stability problems which occur with finite difference methods. However, if the boundary conditions are periodic then the Laplace transform can not be applied directly since Stehfest's numerical inversion technique is unable to cope with the oscillatory nature of the underlying solution. By applying the

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process in a piecewise manner in regions of width $\frac{1}{2}T$, where the period is $2T$, we ensure that the process is applied only over regions where the boundary conditions are monotonic.

An interesting observation is that we must use the process in a piecewise manner of intervals of width one-quarter period. We might expect that we should need only consider intervals of width one-half period. Our numerical experiments [13] show that this is not the case.

There has been little work done to explain the behaviour of the errors in Stehfest's method. More information on the analysis of the Laplace transform inversion errors may enable to attempt an explanation of the nature of the errors in our process for dealing with periodic boundary conditions.

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