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A Hybrid Laplace Transform/Finite Difference Boundary Element Method for Diffusion Problems

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Abstract: The solution process for diffusion problems usually involves the time development separately from the space solution. A finite difference algorithm in time requires a sequential time development in which all previous values must be determined prior to the current value. The Stehfest Laplace transform algorithm, however, allows time solutions without the knowledge of prior values. It is of interest to be able to develop a time-domain decomposition suitable for implementation in a parallel environment. One such possibility is to use the Laplace transform to develop coarse-grained solutions which act as the initial values for a set of fine-grained solutions. The independence of the Laplace transform solutions means that we do indeed have a time-domain decomposition process. Any suitable time solver can be used for the fine-grained solution. To illustrate the technique we shall use an Euler solver in time together with the dual reciprocity boundary element method for the space solution.

Keyword: Boundary element method, finite difference method, diffusion problem

1 Introduction

We consider an approach to the numerical solution of the diffusion problem in which the 'space variation' is developed using a boundary element approach and the 'time development' is obtained in a hybrid Laplace transform/finite difference manner. The motivation for this study is the proposal of a time domain-decomposition procedure which has the potential for exploitation in a parallel computing environment. Such procedures have been considered before in a purely finite difference context Lions (2001); Bal (2002); Maday (2005) in terms of the so-called *parareal algorithm* and this proposed approach is as follows: Decompose the time integration into coarse-grained time slabs and find the solution at the start of each time slab. Now use this coarse solution as an initial-value for a fine-grained solution over each slab. The fine-grained solution can then be used to recalculate the coarse solution and the process repeated. The coarse solution is sequential whereas the fine-grained solutions can be developed in parallel. There is also a potential data-distribution difficulty in the updating of the coarse solution as initial-values for the fine-grained solutions since there is no guarantee that the solutions in different time-slabs would be obtained in synchronisation. This difficulty would be overcome if the coarse solution could also be developed in parallel.

A numerical Laplace transform approach using Stehfest's Stehfest (1970a,b) method provides just such an approach since the solution at any specific time can be obtained independently of those at any other times. The space solution at each time value could be obtained by any suitable solver. The most commonly used approach is that using finite differences Lions (2001); Bal (2002); Maday (2005); Bal (2005), however Cortial and Farhat Cortial (2005) describe an approach using finite elements. In our approach we shall use a boundary element technique in space incorporating the dual reciprocity method. This has been used extensively by the authors in both Laplace transform and finite difference time-decompositions Crann (2005); Crann, Davies, Lan and Leong (1998); Davies and Crann (2001); Davies, Toutip and Bartholomew-Biggs (2001). A discussion of the use of the Stehfest method in

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a boundary element context is given by Sutradhar *et al.* Sutradhar, Paulino and Gray (2002)

We take as our test problem

$$\nabla^2 u = \frac{1}{\alpha}\frac{\partial u}{\partial t} + h(x,y,t) \quad \text{in } \Omega \tag{1}$$

subject to the boundary conditions

$$\begin{aligned} u(s,t) &= u_1(s,t) \quad \text{on } \Gamma_1 \\ q(s,t) &= \frac{\partial u}{\partial n}(s,t) = q_2(s,t) \quad \text{on } \Gamma_2 \end{aligned} \tag{2}$$

$$\text{with } u(x,y,0) = u_0(x,y) \quad \text{in } \Omega \tag{3}$$

where Ω is a closed two-dimensional region bounded by the curve $\Gamma = \Gamma_1 + \Gamma_2$. We seek the solution $u(x,y,t)$ for $(x,y)\varepsilon\,\Omega$ and $0 < t \leq T$.

2 The Hybrid Algorithm

2.1 The Laplace transform

We define the Laplace transform, $\overline{u}(x,y;\lambda)$, of $u(x,y,t)$ as

$$\overline{u}(x,y;\lambda) = \int_0^\infty u(x,y,t)e^{-\lambda t}\,dt$$

Taking the Laplace transform of the initial boundary-value problem (1), (2), (3) we obtain

$$\nabla^2 \overline{u} = \frac{1}{\alpha}(\lambda \overline{u} - u_0) + \overline{h} \quad \text{in } \Omega \tag{4}$$

$$\begin{aligned} \overline{u}(s;\lambda) &= \overline{u}_1(s;\lambda) \quad \text{on } \Gamma_1 \\ \overline{q}(s;\lambda) &= \overline{q}_2(s;\lambda) \quad \text{on } \Gamma_2 \end{aligned} \tag{5}$$

The elliptic boundary-value problem given by equations (4) and (5) is solved using the dual reciprocity method Crann (2005); Zhu (1997) as follows:

We write equation (4) in the form

$$\nabla^2 \overline{u} = b(x,y,\overline{u};\lambda) \quad \text{in } \Omega \tag{6}$$

subject to the same boundary equations (5).

In this form we can apply the dual reciprocity approach using the fundamental solution, u^*, of the Laplacian operator given by

$$u^* = -\frac{1}{2\pi}\ln R \tag{7}$$

Consequently we use the fundamental solution (7) and Green's theorem and write equation (6) in the integral form

$$c_i\overline{u}_i + \int_\Gamma q^*\overline{u}_i\,d\Gamma - \int_\Gamma u^*\overline{q}_i\,d\Gamma + \int_\Omega b_i u^*\,d\Omega = 0 \tag{8}$$

We approximate the source term, b, in equation (6) in terms of a linear combination of radial basis functions, $f_j(R)$, in the form

$$b_i = \sum_{j=1}^{M} \alpha_j f_j(R_i) \tag{9}$$

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 are chosen in such a manner that we can find a particular solution $\hat{u}$ with the property $\nabla^2\hat{u} = f_j$ and we define $\hat{q} = \partial\hat{u}/\partial n$. Using these functions in equation (8) and using Green's theorem we obtain the boundary integral equation

$$\begin{aligned} c_i\overline{u}_i + \int_\Gamma q^*\overline{u}_i\,d\Gamma - \int_\Gamma u^*\overline{q}_i\,d\Gamma \\ = \sum_{j=1}^{N}\alpha_j\left(c_i\hat{u}_{ij} + \int_\Gamma q^*\hat{u}_j\,d\Gamma - \int_\Gamma u^*\hat{q}_j\,d\Gamma\right) \end{aligned} \tag{10}$$

Internal values are given by

$$\begin{aligned} c_i\overline{u}_i = -\int_\Gamma q^*\overline{u}_i\,d\Gamma + \int_\Gamma u^*\overline{q}_i\,d\Gamma \\ + \sum_{j=1}^{L}\alpha_j\left(c_i\hat{u}_{ij} + \int_\Gamma q^*\hat{u}_j\,d\Gamma - \int_\Gamma u^*\hat{q}_j\,d\Gamma\right) \end{aligned} \tag{11}$$

We note here that we could consider the operator in equation (4) to be the modified Helmholtz operator and the associated fundamental solution $u^* = \frac{1}{2\pi}K_0\left(\sqrt{\frac{\lambda}{\alpha}}R\right)$ but there would be no obvious benefit since we would still need a dual reciprocity approach to handle the non-homogeneous term in equation (4).

There has been some recent interest in cases for which there is no convenient analytic form but

where there is the possibility of a numerical computation of the fundamental solution Obreakspace and Duddeck (2006). Also, if the equation contains a convection term then this may be incorporated into the Green's function Simões and Tadeu (2005). The Laplace transform approach is also appropriate in such cases as these.

Equations (10) and (11) may be combined, together with collocation at the M nodes in equation (9), to give the overall set of equations

$$\mathbf{H}\overline{\mathbf{U}} - \mathbf{G}\overline{\mathbf{Q}} = \left[\mathbf{H}\hat{\mathbf{U}} - \mathbf{G}\hat{\mathbf{Q}}\right]\mathbf{F}^{-1}\mathbf{b}(\overline{\mathbf{U}}) \tag{12}$$

where $\mathbf{F}$ is the collocation matrix from equation (9) written in the form $\mathbf{b} = \mathbf{F}\alpha$. Here matrices $\mathbf{H}$ and $\mathbf{G}$ are the usual boundary element matrices and $\hat{\mathbf{U}}$ and $\hat{\mathbf{Q}}$ are the matrices of collocated values of the functions $\hat{\mathbf{u}}$ and $\hat{\mathbf{q}}$ Wrobel (2002).

Equation (12) can be written in the form

$$\mathbf{H}\overline{\mathbf{U}} - \mathbf{G}\overline{\mathbf{Q}} = \mathbf{S}\mathbf{b}(\overline{\mathbf{U}}) \tag{13}$$

where $\mathbf{S}$ is a matrix which depends only on the geometry.

By virtue of the form of equation (4) we see that $\mathbf{b}$ is a linear function of $\overline{\mathbf{u}}$ so that equation (13) is a linear system of equations. The solution of equation (13) yields the approximate transforms $\overline{\mathbf{U}}$ and $\overline{\mathbf{Q}}$ which may then be inverted to obtain the approximate solutions $\mathbf{U}$ and $\mathbf{Q}$.

To implement the Stehfest method 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

$$\left\{\lambda_j = j\frac{\ln 2}{\tau}: \quad j = 1,2,\ldots,m;\ m \text{ even}\right\} \tag{14}$$

The dual reciprocity boundary element method is applied to equation (6) for each λ_j to obtain a set of approximate boundary values

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

and a set of internal values

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

The inverse transforms are then given as follows:

$$U_r = \frac{\ln 2}{\tau}\sum_{j=1}^{m} w_j \overline{U}_{rj} \tag{15}$$

and

$$U^I_r = \frac{\ln 2}{\tau}\sum_{j=1}^{m} w_j \overline{U}_{rj} \tag{16}$$

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

The weights, w_j, are given by Stehfest Stehfest (1970a,b) as

$$w_j = (-1)^{\frac{m}{2}+j} \cdot \sum_{k=[\frac{1}{2}(1+j)]}^{\min(j,\frac{m}{2})} \frac{k^{\frac{m}{2}}(2k)!}{(\frac{m}{2}-k)!\,k!\,(k-1)!\,(j-k)!\,(2k-j)!} \tag{17}$$

2.2 Finite Difference Method

If we define the time slabs as

$$0 = \tau_0 \le t < \tau_1,\ \tau_1 \le t < \tau_2, \ldots, \tau_{p-1} \le t < \tau_p = T$$

then the fine-grained approach is applied in each time slab $\tau_i \le t < \tau_{i+1} \quad (i = 0,1,\ldots,p-1)$ and we could use any suitable finite difference time integration scheme. We shall use the Euler method to illustrate the process; indeed most finite difference- based boundary element processes do use Euler but we may well wish to use a more accurate algorithm such as Runge-Kutta.

We use $n-1$ time steps with time step

$$\Delta t = (\tau_{i+1} - \tau_i)/n$$

The Euler algorithm to solve equation (1) is given by the explicit scheme

$$\nabla^2 u_i^{(k+1)} = \frac{1}{\alpha\Delta t}u_i^{(k+1)} - \frac{1}{\alpha\Delta t}u_i^{(k)} + h(x,y,t_k) \qquad k = 0,1,\ldots,n-1 \tag{18}$$

with

$$t_{k+1} = t_k + \Delta t, \quad t_0 = \tau_i$$

In a similar manner to that in section 2.1 we can develop the dual reciprocity form of equation (18) as

$$\mathbf{H}\mathbf{U}^{(k+1)} - \mathbf{G}\mathbf{Q}^{(k+1)} = \mathbf{S}\mathbf{b}(\mathbf{U}^k) \tag{19}$$

and the solution of this system of linear equations yields the solutions at the times t_k.

3 Examples

Example 1

We consider the problem given by equation (1), with $\alpha = 1$ and $h = 0$, in the unit square $\{(x,y) : 0 \le x \le 1,\ 0 \le y \le 1\}$ subject to the boundary conditions

$$u(x,1,t) = 0 \quad u(1,y,t) = 1$$

$$q(0,y,t) = q(x,0,t) = 0$$

and the initial condition $u(x,y,0) = 0$.

The problem has the analytic solution

$$\begin{aligned} &u(x,y,t) \\ &= 1 - \frac{16}{\pi^2}\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{(-1)^{m+n}}{(2m+1)(2n+1)} \\ &\quad \cdot\cos\left[\frac{(2n+1)\pi x}{2}\right]\times\ldots\ldots\times\cos\left[\frac{(2m+1)\pi y}{2}\right] \\ &\qquad \cdot\exp\left(-\alpha\pi^2\left[(2m+1)^2+(2n+1)^2\right]t/4\right) \end{aligned}$$

We use 36 linear boundary elements with 9 internal nodes. The radial basis functions for the dual reciprocity method are given by $f_j(R) = 1 + R$.

The coarse-grained Laplace transform solution is developed at $t = 0.2, 0.4, \ldots, 1$ *i.e.* over equal time slabs, and the fine-grained Euler solver uses a time step $\Delta t = 0.025$. The solution is shown in figure 1.

We see that the hybrid Laplace transform/Euler method compares well with the analytic solution. We note that the Laplace transform solution at $(0.75, 0.75)$ with $t = 0.2$ is relatively poor. This reflects the relatively low value, $\tau = 0.2$, in equation (14); it is well-documented Crann (2005) that Stehfest's method can yield relatively poor values for small values of τ. It is interesting to note that, even though the Laplace transform value at

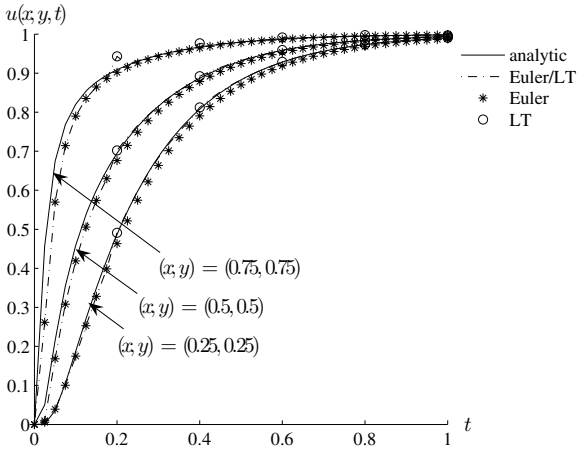

Figure 1: Solution to the problem in example 1 at three points for $0 \le t \le 1$.

$t = 0.2$ is relatively poor, we still obtain good results from the Euler solver in $0.2 < t < 0.4$.

A parallel algorithm is potentially of most use in non-linear problems. To illustrate we consider the following example.

Example 2

We consider the problem

$$\nabla^2 u = \frac{1}{\alpha}\frac{\partial u}{\partial t} + u^2 + h(y,t)$$

with $\alpha = 1$, defined in the unit square $\{(x,y) : 0 \le x \le 1,\ 0 \le y \le 1\}$ subject to the boundary conditions $u(0,y,t) = 0$, $u(1,y,t) = t^2$, $q(x,0,t) = q(x,1,t) = 0$ and the initial condition $u(x,y,0) = u_0(x,y) = 0$ with $h(x,y,t) = 2t^2 - 2x^2t$. The problem has the analytic solution $u = x^2t^2$.

We use 36 linear boundary elements with 9 internal nodes for the dual reciprocity method. The radial basis functions are $f_j(R) = 1 + R$. The Laplace transform solution is developed at times $0.5p$ $(p = 1, 2, \ldots, 8)$ and the Euler time step is $\Delta t = 0.1$ in each time slab.

In this case we cannot apply the Laplace transform directly due to the non-linear term u^2. We use a direct iteration approach Crann (2005) in which we write the partial differential equation in the form

$$\nabla^2 u_i = \frac{1}{\alpha}\frac{\partial u_i}{\partial t} + u_{i-1}^2 + h(x,y,t) \qquad i = 1, 2, \ldots,$$

with $u^{(0)} = u_0$.

The Laplace transform approach gives

$$\nabla^2 \overline{u}_i = \frac{1}{\alpha}(\lambda \overline{u}_i - u_0) + \frac{u_{i-1}^2}{\lambda} + \overline{h}(x,y;\lambda)$$

Again, in each iteration, this equation is of the same form as equation (6) and the dual reciprocity equations are of the same form as equation (13). The explicit Euler algorithm solver requires only a simple modification of equations (18) and (19).

In figure 2 we show the time development at the points $(0.2,0.2)$, $(0.5,0.5)$, $(0.8,0.8)$ for $0 \leq t \leq 4$. On this scale we are unable to see how the solution has developed. Consequently we consider the time development at the point $(0.8,0.8)$ for $3 \leq t \leq 4$ and this is shown in figure 3.

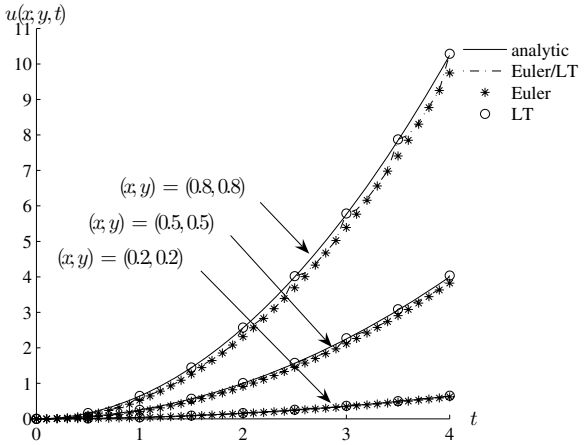

Figure 2: Time development of the solution at three points for $0 \leq t \leq 4$.

From figure 3 we see that the Laplace transform solution, the coarse-grained solution, compares well with the analytic solution. The Euler solution is diverging from the analytic solution as time progresses. The hybrid Laplace transform/finite difference solution (LT/FDM) does not deteriorate as time progresses. However, the fine-grained Euler solution is progressively worse as time progresses. In order to illustrate this phenomenon we calculate the difference between the RMS errors for the Euler/Laplace transform method, e_{ELT}, and for the Euler method, e_E. This difference, $e_E - e_{ELT}$ is shown in figure 4.

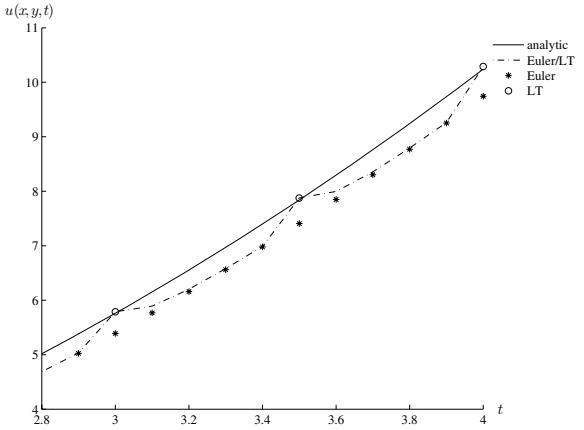

Figure 3: Time development of the solution at the point $(0.8,0.8)$ for $3 \leq t \leq 4$.

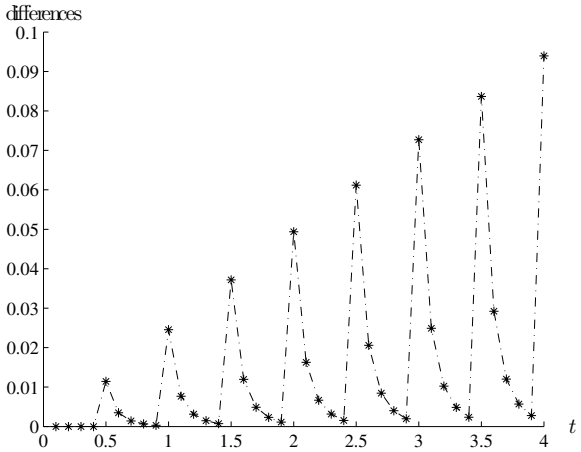

Figure 4: Difference between the RMS errors for $0 \leq t \leq 4$.

We notice from figure 4 that $e_E - e_{ELT}$ is positive and that it has its maximum at time τ_i, the beginning of time slab i, where the coarse-grained Laplace transform solution 'pulls' the fine-grained Euler back towards the analytic solution. We notice also that these differences increase as t increases.

In this example we have chosen a relatively large time-step for the fine-grained solver to show how the relatively accurate coarse-grained solver acts to mitigate the errors. In practice of course we would use a fine-grained step-size so that the order of error within each time slab is at least of the same order as the coarse-grained solver. In figure 5 we show the hybrid LT/FDM for time slabs of

size 0.2 and an Euler step size $\Delta t = 0.01$.

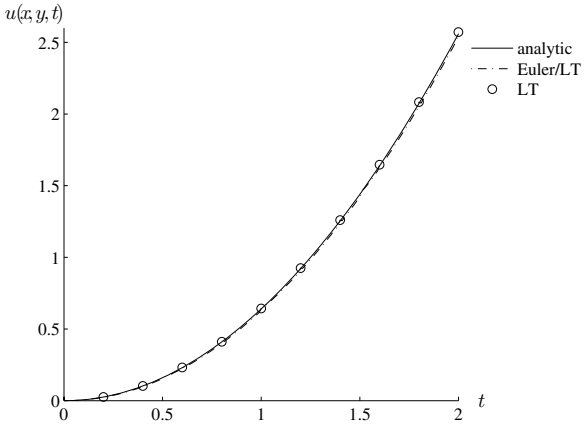

Figure 5: Time development of the solution at $(0.8, 0.8)$.

4 Conclusions

The hybrid Laplace transform/finite difference method provides a suitable approach to the solution of diffusion problems. In this investigation we have considered the approach in a sequential manner. The process is, however, inherently parallel; the fine-grained solutions could all be obtained independently. Also, there would be no inter-processor communication and the implementation would have an excellent load balance since each processor performs exactly the same program on the same amount of data.

There is an important consideration in respect of the errors in the Laplace transform; the coarse-grained solution must be of the same order of accuracy as the fine-grained solution. Convergence criteria and error bounds for finite difference algorithms are well-documented Lambert (1983). However the behaviour of errors in the Stehfest Laplace transform method are not explicitly available; clearly until such theory is available it is difficult to make specific judgements on how to implement the hybrid method. In practice, of course, it is the overall error which is important and it is quite likely that so long as the Laplace transform solution is sufficiently accurate the fine-grained solver can be implemented in such a way that the solution over each time slab is no worse than the coarse-grained solution. It is important to notice that in a parallel environment we can afford to do as much work in each time slab as would be needed in a global solution with the same finite difference approach to yield at least an accurate solution as that produced by the coarse-grained, Laplace transform, solution.

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