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The method of fundamental solutions for time-dependent problems

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Abstract

1 Introduction

Boundary methods for solving elliptic particular differential equations have become well established tools for solving many problems of engineering science. In particular, Trefftz-type methods such as the method of fundamental solutions(MFS) have become increasingly popular over the past decade [1, 2]. However, for parabolic and hyperbolic equations the situation is less satisfactory and boundary methods for these equations seen to be less developed. A major difficulty is that the traditional formulations usually require the evaluation of numerous domain integrals which can be time consuming to compute. One way around this is to use Dual Reciprocity techniques which can be effective, but cumbersome [3]. Until recently, no boundary-only formulations appeared to be available for this class of problems. In this paper we develop an approach to solving a variety of time-dependent problems which requires neither domain nor boundary discretization by coupling the MFS with recently derived particular solutions for the inhomogeneous Helmholtz equation with thin plate and higher order splines as right hand sides.

Our algorithms proceed by showing how boundary value problems for a variety of time-dependent partial differential equations can be reduced to solving boundary value problems for inhomongeneous Helmholtz-type equations. Using the particular solutions derived in [4], these inhomogeneities

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can be eliminated. The resulting homogeneous equations can then be solved using a variety of boundary methods. As we show, the MFS is a highly efficient method for doing this.

Two approaches are given for reducing the time-dependent problems to time-independent ones: Laplace transforms and finite differencing in time. In Section 2 we apply these methods to the diffusion equations in $\mathbb{R}^d, d = 2, 3$ and this is followed in Section 3 by a discussion of methods for computing particular solutions to the inhomogeneous Helmholtz equation. In Section 4 we show how to extend these techniques to solve the wave equation and in Section 5 we generalize a scheme of Tabarrok and Su [5] to solve the convection-diffusion equation and a class of semilinear diffusion equations.. We close with some preliminary numerical results in Section 6.

2 The diffusion equation

As motivation for our work we consider boundary value problems for the diffusion equation

$$\Delta u(P,t) - u_t(P,t) = f(P,t), \quad P \in D \subseteq \mathbb{R}^d, \quad d = 2,3 \tag{1}$$

where D is a bounded domain in $\mathbb{R}^d, d = 2, 3$. For simplicity, we assume Dirichlet boundary conditions

$$u(P,t) = g(P,t), \quad P \in \partial D, \quad t > 0 \tag{2}$$

and the initial condition

$$u(P,0) = h(P), \quad P \in D. \tag{3}$$

As is well known, the initial boundary value problem (IBVP) (1)-(3) has a unique solution under quite general conditions on (f, g, h) and ∂D [6].

To solve (1)-(3) numerically, we consider two approaches: (i) taking the Laplace transform in 't' [7] and (ii) finite differencing in 't' [8]. Defining the Laplace transform

$$\hat{u}(P,s) = \int_0^\infty e^{-st} u(P,t)dt, \quad s > M \tag{4}$$

and applying (4) to (1)-(3) $\hat{u}$ satisfies the boundary value problem

$$\begin{aligned} \Delta\hat{u}(P,s) - s\hat{u}(P,s) &= \hat{f}(P,s) - h(P) \equiv m(P,s) && (5)\\ \hat{u}(P,s) &= g(P,s), \quad P \in \partial D. && (6) \end{aligned}$$

If $m(P,s) \neq 0$, then (5) is an inhomogeneous modified Helmholtz equation. Defining $v = \hat{u} - u_p$ where u_p is a particular solution to (5), v satisfies

$$\begin{aligned} \Delta v(P,s) - sv(P,s) &= 0, \quad P \in \partial D, && (7)\\ v(P,s) &= g(P,s) - u_p(P,s), \quad P \in \partial D. && (8) \end{aligned}$$

Equations (7)-(8) can now be solved by using boundary methods such as the MFS [1].

In the MFS we approximate the solution to (7) by

$$v(P,s) \simeq v_n(P,s) = \sum_{k=1}^{n} a_k G(P, Q_k; s) \tag{9}$$

where $G(P,Q;s)$is the fundamental solution for $\Delta - s$ [7] and $\{Q_k\}_1^n$ are source points on a fictitious surface S containing D. Typically, $\{a_k\}_1^n$ are determined by collocation by setting

$$\sum_{k=1}^{n} a_k G(P_j, Q_k; s) = g(P_i, s) - u_p(P_i, s), \quad 1 \le j \le n, \tag{10}$$

where $\{P_j\}_1^n$ are n distinct points on ∂D. (Although we have not done so in our work, least squares techniques for choosing $\{a_k\}_1^n$ and $\{Q_k\}_1^n$, can also be used [2].) Having determined v_n,an approximation to $\hat{u}$ is given by

$$\hat{u}_n = v_n + u_p. \tag{11}$$

We then obtain an approximation u_n to u by numerical inversion of $\hat{u}_n$. Following work by Zhu [9] we have found Stehfest's algorithm [10] to be an effective method for this purpose.

To complete the algorithm we need to determine u_p. In general, this cannot be done explicitly, so a further numerical approximation is necessary. In [11] we used an idea of Atkinson to do this. As observed in [11] a particular solution to (5) is given by

$$u_p(P,s) = \int_{\hat{D}} G(P,Q;s) m(Q,s) dv \tag{12}$$

where $\hat{D}$ is a domain containing D in its interior. Choosing $\hat{D}$ to be a circle in $\mathbb{R}^2$ or a sphere in $\mathbb{R}^3$ (12) can be reduced to an integral which can be evaluated by standard numerical methods [11]. Although this approach is effective, it can be inefficient, particularly in $\mathbb{R}^2$ where $G(P,Q;s)$ is a Bessel function [11].

To improve the efficiency of the algorithm in [11] we considered using a DRM-type technique by approximating $m(P,s)$ in (5) by thin plate splines [7]. In contrast to the classical $1+r$ basis, in this case one can obtain the particular solutions analytically using a generalization of the annihilator method used to obtain particular solutions for ordinary differential equations [12]. In [7] we showed how to extend this argument to analytically calculate particular solutions when higher order polynomial splines are used as basis elements. This will be discussed further in the following section.

Because numerical inversion of the Laplace transform is an ill-posed problem, the above algorithm may not be effective for all problems. To

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overcome this difficulty, one can proceed by using finite differences rather than the Laplace transform in time. A popular class of methods for doing this are the θ-methods defined as follows [3]: let $\tau > 0$ and define the mesh $t_n = n\tau, n \geq 0$. For $t_n \leq t \leq t_{n+1}$, approximate $u(P,t)$ by $(0 \leq \theta \leq 1)$

$$u(P,t) \simeq \theta u(P,t_{n+1}) + (1-\theta)u(P,t_n) \quad (13)$$

$$\Delta u(P,t) \simeq \theta \Delta u(P,t_{n+1}) + (1-\theta)\Delta u(P,t_n) \quad (14)$$

and

$$u_t \simeq \frac{u(P,t_{n+1}) - u(P,t_n)}{\tau}. \quad (15)$$

Using (14)-(15) in (1) and denoting the resulting approximation to $u(P,t_n) \equiv u_n(P)$ by $v_n(P)$, v_n satisfies

$$\theta \Delta v_{n+1} + (1-\theta)\Delta v_n - \frac{(v_{n+1} - v_n)}{\tau} = f_n \quad (16)$$

so that $(f_n \equiv f(P,t_n))$

$$\Delta v_{n+1} - \frac{v_{n+1}}{\theta\tau} = \frac{-v_n}{\theta\tau} - \frac{(1-\theta)\Delta v_n}{\theta\tau} + f_n. \quad (17)$$

For $\theta = 1$ we get the backward difference scheme (sometimes called Rothe's method [8])

$$\Delta v_{n+1} - \frac{v_{n+1}}{\tau} = \frac{-v_n}{\tau} + f_n \quad (18)$$

and for $\theta = 1/2$ we get the Crank-Nicholson scheme

$$\Delta v_{n+1} - \frac{2v_{n+1}}{\tau} = \frac{-2v_n}{\tau} - \Delta v_n + 2f_n. \quad (19)$$

Now observe that (17) is a sequence of inhomogeneous modified Helmholtz equations which can be solved using $v_0 = h$ and the boundary conditions $v_n(P) = g(P,t_n), P \in \partial D$. As before, v_{n+1} can be determined using the MFS once the right hand side of (17) is known. Particular solutions can then be determined using either Atkinson's formula (12) or approximations using higher order splines. We turn to this next.

3 Particular solutions for polyharmonic splines

As shown above our approach to solving the diffusion equation requires one to be able to calculate particular solutions for the operator $\Delta - \lambda^2$ for appropriately chosen right hand sides. Traditionally in the DRM one has used $1 + r$ basis functions for this purpose [3]. However, in this case closed form particular solutions are not available [13] and so other choices need to be considered. In [12] it was shown that closed form solutions could

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be obtained for thin plate splines and in [4] this was generalized to higher order polyharmonic splines. Since those functions can provide arbitrarily high orders of approximation, they appear to be very suitable for numerical work. For completeness we give an overview of these results here.

Hence, we consider solving

$$\Delta\psi - \lambda^2\psi = f \tag{20}$$

where f is a polyharmonic spline; i.e.,

$$f(P) = \sum_{j=1}^{N} a_j \varphi_j^{[n]}(r_j) + p_n \tag{21}$$

where

$$\varphi_j^{[n]}(r_j) = \begin{cases} r_j^{2n}\log r_j, & n \geq 1, \quad \text{in } \mathbb{R}^2 \\ r_j^{2n-1}, & n \geq 1, \quad \text{in } \mathbb{R}^3 \end{cases} \tag{22}$$

Here p_n is a polynomial of degree n, $r_j = \|P - P_j\|$ and $\{P_j\}_1^N$ is a unisolvent set of points for polynomial interpolation. In addition, if $\{a_j\}_1^N$ satisfy

$$\sum_{j=1}^{N} a_j b_i(P_j) = 0, \quad 1 \leq i \leq l_n, \tag{23}$$

where $\{b_j\}_1^{l_n}$ is a basis for the polynomials of deg $\leq n$, then for a given f there is a unique polyharmonic spline interpolant $\hat{f}$ of the form (21) on $\{P_j\}_1^N$. For a smooth f one can show that [14]

$$\left\| f - \hat{f} \right\|_2 \leq ch^n \tag{24}$$

where h is the mesh width of $\{P_j\}_1^N$.

Hence, to obtain approximate particular solutions to $(\Delta - \lambda^2)u_p = f$ we approximate f by $\hat{f}$ and solve $(\Delta - \lambda^2)\hat{u}_p = \hat{f}$. By linearity, it suffices to solve

$$(\Delta - \lambda^2)\psi_j^{[n]} = \varphi_j^{[n]}. \tag{25}$$

In [4] it was shown that $\psi_j^{[n]}$ was of the form $\psi_j^{[n]} = \psi^{[n]}(r_j)$ where

$$\psi^{[n]}(r) = \begin{cases} AI_0(\lambda r) + BK_0(\lambda r) + \sum_{k=1}^{n+1} c_k r_j^{2k-2}\log r + \sum_{k=1}^{n+1} d_k r^{2k-2} & \text{in } \mathbb{R}^2, \\ \dfrac{A\cosh(\lambda r)}{r} + \dfrac{B\sinh(\lambda r)}{r} + \sum_{k=-1}^{n} a_k r^k & \text{in } \mathbb{R}^3, \end{cases} \tag{26}$$

where the coefficients in (26) are chosen to guarantee maximal smoothness of $\psi^{[n]}$ at $r = 0$. Details and proofs are given in [4].

4 The wave equation

Although much of the BEM literature on time-dependent problems is devoted to parabolic equations, there is a growing literature on hyperbolic problems, particularly the wave equation [15]. Here we show how the approach in Section 2 can be extended to this class of problems.

Hence, we consider the IBVP

$$\Delta u(P,t) = u_{tt}(P,t), \quad P \in D, \quad t > 0 \tag{27}$$
$$u(P,0) = u_0, \quad u_t(P,0) = v_0 \tag{28}$$

with, for example, Dirichlet boundary conditions

$$u(0,t) = g(P,t), \quad P \in \partial D, \quad t > 0. \tag{29}$$

If one takes the Laplace transform of (27), then the Laplace transform $\hat{u}$ of u satisfies

$$\Delta \hat{u}(P,s) = s\hat{u}(P,s) - su_0 - v_0, \quad P \in D, \tag{30}$$
$$\hat{u}(P,s) = \hat{g}(P,s) \quad P \in \partial D. \tag{31}$$

From (30) we see that $\hat{u}$ satisfies an inhomogeneous modified Helmholtz equation so the determination of $\hat{u}$ proceeds as for the diffusion equation. To obtain an approximation in 't' one needs to invert the numerical approximation to $\hat{u}$. For this, Stehfest's algorithm may not appropriate and we are currently investigating a number of alternatives [18].

To avoid transform inversion problems one can resort to time-differencing as for the diffusion equation. Generalizing the approach of Su and Tabarrok [5] one can define a class of θ algorithms as follows: approximate u_{tt} by the central difference formula ($u_n \equiv u(P,t_n)$)

$$u_{tt} \simeq \frac{u_{n+1} - 2u_n + u_{n-1}}{\tau^2} \tag{32}$$

and

$$(\Delta u)_n \simeq \theta\,(\Delta u)_{n+1} + (1-\theta)\,(\Delta u)_{n-1}\,. \tag{33}$$

Substituting (32) and (33) into (27) and denoting the resulting approximation to u_n by v_n, it satisfies

$$\theta \Delta v_{n+1} - \frac{v_{n+1}}{\tau^2} = \frac{v_{n-1} - 2v_n}{\tau^2} + (1-\theta)\Delta v_{n-1}. \tag{34}$$

For $\theta = 1/2$ we get a second order accurate Crank-Nicholson scheme [5].

Again we see for $\theta \neq 0$ that v_n satisfies a sequence of inhomogeneous Helmholtz equations which can be solved in the same fashion as for the diffusion equation.

5 The convection-diffusion equation

When the differential equation has non-constant coefficients and/or is non-linear, then transform methods generally fail. However, time-differencing can still lead to useful algorithms [5]. Here we illustrate this for the convection-diffusion equation and a class of semilinear diffusion equations.

The convection-diffusion equation is of the form

$$\Delta u = \sigma\vec{V} \cdot \nabla u + u_t \tag{35}$$

where $\vec{V}$ is a (possibly non-constant) 'velocity' field, ∇u is the gradient of u and '$\cdot$' the usual dot product in $\mathbb{R}^d, d = 2,3$. If one approximates u_t by the central difference formula

$$u_t \simeq \frac{u_{n+1} - u_{n-1}}{2\tau} \tag{36}$$

and Δu as in (33), then substituting this into (27), the approximation v_n to u_n satisfies

$$\theta\Delta v_{n+1} + (1-\theta)\Delta v_{n-1} - \frac{1}{2\tau}(u_{n+1} - v_{n-1}) = \sigma\vec{V} \cdot \nabla u. \tag{37}$$

On rearrangement (37) again is seen to be a sequence of inhomogeneous Helmholtz equations which can be solved using the MFS as before.

We note that if the convection term $\sigma\vec{V} \cdot \nabla u$ is replaced by a general nonlinear term of the form $f(P, u, \nabla u)$ then the scheme given above can be implemented to solve the nonlinear diffusion equation

$$\Delta u(P,t) - u_t(P,t) = f(P, \nabla u, u). \tag{38}$$

Interestingly, this scheme requires no spatial iteration in contrast to the steady state case $u_t = 0$ [17].

6 A numerical example

To illustrate some of these ideas numerically, we consider the following boundary value problem for the diffusion equation:

$$\frac{1}{k}\Delta u(P,t) = u_t(P,t), \quad P = (x,y) \in D, \quad t > 0, \tag{39}$$

$$u(P,t) = 0, \quad P \in \partial D, \tag{40}$$

$$u(P,t) = 1, \quad P \in D, \tag{41}$$

where $D = (-0.2, 0.2) \times (-0.2, 0.2)$ and $k = 5.8 \times 10^{-3}$. The analytic solution to (39)-(41) was given by Carslaw and Jaeger in [18].

To solve (39)-(41) we use the backward difference scheme (18) with $\tau = 0.025$ and time interval $(0, 0.9]$. To approximate the right hand sides in

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(18) we used polyharmonic splines of order $n = 1$ to $n = 4$. For interpolation we chose 25 points uniformly distributed in D and 16 points uniformly distributed on ∂D. To solve the homogeneous equation, the MFS was used with 16 source points uniformly distributed on a circle of radius three containing D and 16 collocation points uniformly distributed on ∂D. In Table 1 are shown the % relative errors of the solution at six interior points in $[0, 0.2] \times [0, 0.2]$ ($S_n, 1 \leq n \leq 4$ denote splines of order n. Here $n = 1$ are thin plate splines.). One should note the substantial increase in accuracy as the order of splines increases.

Table 1. Relative errors (%) at six interior points.

x	y	TPS	S2	S3	S4
0.00	0.00	3.93	1.70	1.35	1.01
0.10	0.00	8.00	1.71	0.83	0.40
0.10	0.10	11.50	2.07	0.34	0.39
0.05	0.05	6.04	1.69	1.09	0.68
0.05	0.15	13.00	2.44	0.11	0.58
0.15	0.15	13.47	0.53	1.44	0.49

7 Conclusions

We have shown how a number of second order time-dependent partial differential equations can be solved numerically by reformulating them in terms of inhomogeneous modified Helmholtz equations. Using recently derived analytic particular solutions for these equations the resulting boundary value problems can be reduced to solving a homogeneous Helmholtz equation which can be done effectively using the MFS. The resulting algorithms are efficient in that they require neither domain nor boundary discretization. Future work will be devoted to futher numerical experimentation and convergence analysis to enable one to choose the various parameters in a more systematic fashion.

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