

PARTICULAR SOLUTIONS METHODS FOR FREE AND MOVING BOUNDARY PROBLEMS

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1 Introduction

Consider a quasilinear partial differential equation

$$(1) \quad Lu = f \quad \text{on } S$$

subject to a fixed boundary condition

$$(2) \quad B_1 u = g \quad \text{on } \Gamma$$

where Γ is the boundary of the region S . Suppose that u is approximated in the form

$$(3) \quad u \simeq u_n = \sum_{j=1}^n c_j \psi_j(x, y)$$

where ψ_j is a particular solution of Eq. 1 for every j . Suppose that the parameters c_j in Eq. 3 are determined by requiring that u_n should satisfy Eq. 2 approximately according to a chosen interpolation or least squares (or similar) fitting criterion.

In the case of a free boundary problem, the boundary Γ is unknown, and a second boundary condition

$$(4) \quad B_2 u = h \quad \text{on } \Gamma$$

is specified. Some form of iterative procedure is then applied to determine a u_n of form Eq. 3 and an approximation Γ_n to Γ such that, in the limit, u_n satisfies both Eq. 3 and Eq. 4.

Such a “method of particular solutions” has been adopted successfully for free boundary problems by [6], and the aim of the present paper is to expose and further expand on this work. In particular a broader variety of particular solutions is provided, and a wider range of test problems is considered. Specifically a family of piecewise polynomial solutions of the heat equation, which coincide with a spline in t on $x = \pm 1$, is introduced, which provides a robust basis for Stefan and related problems. Further, an advection-diffusion (bush-fire) problem is tackled, using separable variable solutions based on modified Bessel functions and a least squares fitting method on the boundary.

Collocation methods are illustrated in a number of effective applications, but, by way of a cautionary tale, an example is given in which an apparently well chosen collocation method leads to divergent approximations while a least squares method converges.

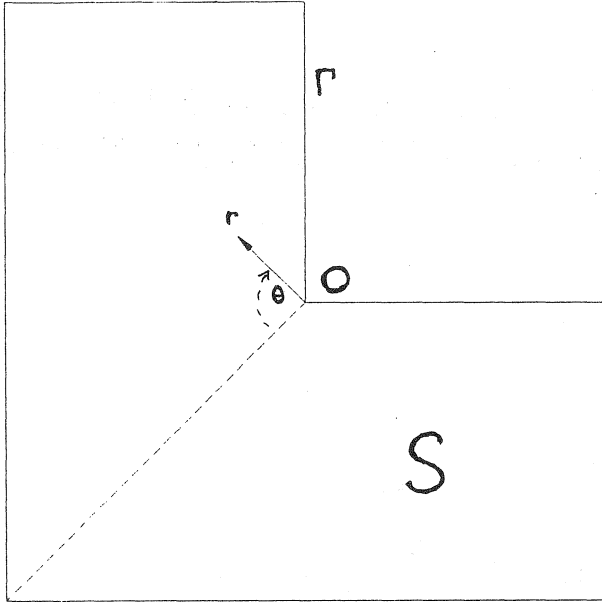


Figure 1: The L-shaped region

2 A Milestone in Particular Solutions

In advocating particular solutions methods, it behoves us to acknowledge our great debt to [4], who demonstrate most elegantly the formidable efficiency that can sometimes be achieved. They consider the vibrating membrane eigenvalue problem

$$(5) \quad \nabla^2 u + \lambda u = 0 \quad \text{in } S$$

$$(6) \quad u = 0 \quad \text{on } \Gamma$$

for the particular case in which S is an L-shaped region consisting of three squares placed together (Figure 1). By separating r, θ variables, and considering even solutions (1st, 3rd, ... eigenvalues), particular solutions are found in the form

$$(7) \quad \psi_j(r, \theta) = J_\alpha(r\sqrt{\lambda}) \cos \alpha \theta$$

for $\alpha = \alpha_j = \frac{2}{3}(2j - 1)$ ($j = 1, 3, 4, 6, 7, \dots, 3k, 3k + 1, \dots$). (Values $j = 2, 5, 8, \dots, 3k + 2, \dots$ are omitted, since these give integral values of α). The functions Eq. 7 are polynomials in $r^{2/3}$ and have precisely the right singular behaviour at the reentrant corner ($r = 0$). Following [5], who extended the accuracy of the FHM results, both an eigenvalue λ and corresponding coefficients c_j in the approximation

$$(8) \quad u_n = \sum_{j=1}^N c_j \psi_j(r, \theta) \quad (j \neq 3k + 2, k \text{ integral})$$

are determined by interpolating Eq. 6 at the zeros of $\cos \alpha_{N+1} \theta$, namely the equal angles

$$(9) \quad \theta = \frac{3\pi}{4} \left(\frac{k - 1/2}{N + 1/2} \right) \quad (k = 1, \dots, N).$$

Only values of θ between $\pi/4$ and $3\pi/4$ are included, as a consequence of the symmetries of the region. Precisely n homogeneous equations are obtained in the n non-zero parameters c_j of Eq. 8, provided we choose

$$(10) \quad N = [3n/2],$$

The equations form a generalised eigenvalue problem, and each eigenvalue may be determined to correspond to a unique (apart from a multiplicative constant) set c_j . Remarkable results are obtained in this way by [5] and in particular, for $n = 24$, the first eigenvalue λ is obtained to what are believed to be 13 correct digits, namely

$$(11) \quad \lambda = 9.639723844022.$$

This example teaches us that if key features of a problem (such as singularities) are included in particular solutions, then a very powerful numerical method may result.

3 Choice of Particular Solutions

There are a variety of possible ways of generating particular solutions, of which we mention four below, and in particular we present a novel family of piecewise polynomial solutions of the heat equation.

3.1 Separation of Variables

In the classical method of separation of variables, solutions are sought as products of functions of one variable, and, since these are by definition particular solutions, they may serve as basis functions for our method. For example the separable variable solutions Eq. 7 were used in the solution of the membrane eigenvalue problem Eq. 5. Some boundary conditions of the problem are generally included, and, for example, Eq. 6 ($u = 0$ on $\theta = \pm 3\pi/4$) is satisfied by Eq. 7.

If odd solutions, corresponding to 2nd, 4th, ... eigenvalues are required, then we replace Eq. 7 by the particular solutions.

$$(12) \quad J_\alpha(r\sqrt{\lambda}) \sin \alpha\theta$$

for $\alpha = \beta_j = \frac{4}{3}j\pi$, ($j = 1, 2, \dots$) which also satisfy the boundary condition Eq. 6.

The one-dimensional heat equation

$$(13) \quad u_{xx} = u_t$$

has classical separable variable solutions

$$(14) \quad \begin{Bmatrix} \cos \alpha x \\ \sin \alpha x \end{Bmatrix} e^{-\alpha^2 t}$$

which may be adopted as transient particular solutions. These are particularly useful in fitting homogeneous boundary conditions such as

$$(15) \quad \lambda u \pm \mu u_x = 0 \quad \text{on } x = \pm 1.$$

and, for example for $\lambda = 1, \mu = 0$ we adopt

$$\begin{aligned} \cos \alpha x & \text{ for } \alpha = \alpha_j = \left(j - \frac{1}{2}\right)\pi, \\ \sin \alpha x & \text{ for } \alpha = \beta_j = j\pi. \end{aligned}$$

However, the solutions Eq. 14 are not appropriate for all boundary conditions and indeed have little relevance to Stefan problems whose solutions grow with time. On the other hand, they are useful as complementary solutions, which, when combined with dominant solutions, may be able to match the boundary conditions - this idea is exploited in §3.4 below.

Either cartesian or polar coordinates may be adopted and lead to particular solutions of rather different characters. For example, Laplace's equation

$$(16) \quad \nabla^2 u = u_{xx} + u_{yy} = r^2 u_{rr} + r u_r + u_{\theta\theta} = 0$$

has as separable variable solutions not only

$$(17) \quad \begin{Bmatrix} \sin \alpha x \\ \cos \alpha x \end{Bmatrix} \cdot \begin{Bmatrix} \sinh \alpha y \\ \cosh \alpha y \end{Bmatrix}$$

but also

$$(18) \quad r^{\pm\alpha} \begin{Bmatrix} \cos \alpha\theta \\ \sin \alpha\theta \end{Bmatrix}.$$

Solutions Eq. 17 may be appropriate to regions bounded by lines parallel to the y axis, and solutions Eq. 18 may be appropriate to regions with corners (α not an integer) or to regions with an interior origin (α an integer).

3.2 Harmonic Functions

Laplace's equation Eq. 16 is almost unique (apart from related equations such as the biharmonic equations) in its close link with complex variable theory. As a consequence of the Cauchy-Riemann equations, the real and imaginary parts of any analytic function are harmonic functions (i.e. solutions of Eq. 16), and this immediately leads to a source of particular solutions. For example, harmonic polynomials are defined as the real and imaginary parts of

$$(19) \quad z^k = (x + iy)^k \quad (k = 0, 1, 2, \dots)$$

i.e.

$$(20) \quad 1; \quad x, \quad y; \quad x^2 - y^2, \quad 2xy; \quad x^3 - 3xy^2, \quad 3x^2y - y^3; \quad \dots$$

In fact, if we change to polar variables then we note that these are just separable variables solutions of form Eq. 18, namely

$$(21) \quad 1; \quad r \cos \theta, \quad r \sin \theta; \quad r^2 \cos 2\theta, \quad r^2 \sin 2\theta; \quad r^3 \cos 3\theta, \quad r^3 \sin 3\theta; \quad \dots$$

Harmonic functions are particularly useful in perfect fluid flow, since both the fluid potential ϕ and the stream function ψ satisfy the Cauchy-Riemann equations and are hence harmonic.

3.3 Special Polynomial Solutions

It is sometimes possible to generate particular solutions by substituting a chosen simple form into a differential equation. For example, for the heat equation Eq. 13, [6] introduce polynomial solutions u of the form

$$(22) \quad P_{2j}(x, t) = \sum_{r=0}^j A_r(x) t^r$$

by specifying

$$(23) \quad u = t^j \quad \text{on } x = \pm 1.$$

This leads to the formulae

$$(24) \quad A_r(x) = \sum_{s=0}^{j-r} a_{sr} x^{2s}$$

where

$$2s(2s - 1) a_{sr} = (r + 1) a_{s-1, r+1}$$

and

$$a_{0j} = 1, \quad a_{0r} = -(a_{1r} + a_{2r} + \dots + a_{j-r, r}).$$

The resulting polynomials are even, of degree $2j$ in x and of degree j in t .

Odd solutions of Eq. 12 may be similarly defined in the form

$$(25) \quad P_{2j+1}(x, t) = \sum_{r=0}^j B_r(x) t^r$$

by specifying

$$(26) \quad u = \pm t^j \quad \text{on } x = \pm 1 \quad (\textit{respectively}).$$

This leads to the formulae

$$(27) \quad B_r(x) = \sum_{j=0}^{s-r} b_{sr} x^{2s+1}$$

where

$$(28) \quad (2s+1)2s b_{sr} = (r+1)b_{s-1, r+1}$$

and

$$(29) \quad b_{0j} = 1, \quad b_{0r} = -(b_{1r} + b_{2r} + \dots + b_{j-r, r}).$$

Specific examples of these even/odd solutions of Eq. 12 are

$$(30) \quad P_6(x, t) = t^3 + t^2 \left(-\frac{3}{2}x + \frac{3}{2}x^2 \right) + t \left(\frac{5}{4} - \frac{3}{2}x^2 + \frac{1}{4}x^4 \right) + \left(-\frac{61}{120} + \frac{5}{8}x^2 - \frac{1}{8}x^4 + \frac{1}{120}x^6 \right)$$

$$(31) \quad P_5(x, t) = t^2 x + t \left(-\frac{1}{3}x + \frac{1}{3}x^3 \right) + \left(\frac{7}{180}x - \frac{1}{18}x^3 + \frac{1}{60}x^5 \right)$$

Such solutions have the advantage of being unbounded in t and are hence used to great effect to solve a Stefan problem in § 6.1 below.

3.4 Piecewise Particular Solutions

Piecewise approximations are known to be advantageous for covering a large region effectively, and it is actually possible to develop piecewise particular solutions, as we now show for the heat equation Eq. 12. For simplicity we shall restrict discussion to even solutions; odd solutions can be developed in a similar way, and hence general solutions can be obtained by combining even and odd parts.

Assume that a general solution $u(x, t)$ coincides on $t = \pm 1$ with the cubic spline

$$(32) \quad S(t) = \sum_{i=0}^3 c_i t^i + \sum_{j=1}^m d_j (t - t_j)_+^3 \quad (0 \leq t \leq T)$$

where

$$(33) \quad (t - t_j)_+^3 = \begin{cases} (t - t_j)^3 & t \geq t_j \\ 0 & t \leq t_j \end{cases}$$

with knots t_1, t_2, \dots, t_m .

Then we may write

$$(34) \quad u(x, t) = u^{(j)}(x, t) \quad \text{on } t_j \leq t \leq t_{j+1}$$

where

$$t_0 = 0, \quad t_{m+1} = T.$$

Clearly

$$(35) \quad u^{(0)}(\pm 1, t) = \sum_{i=0}^3 c_i t^i \quad \text{on } x = \pm 1,$$

and hence

$$(36) \quad u^{(0)}(x, t) = \sum_{i=0}^3 c_i P_{2i}(x, t)$$

where P_{2i} is given by Eq. 22.

Now

$$u^{(j)}(\pm 1, t) = u^{(j-1)}(\pm 1, t) + d_j(t - t_j)^3$$

and hence

$$(37) \quad u^{(j)}(x, t) = u^{(j-1)}(x, t) + d_j Q_j(x, t)$$

where $Q_j(x, t)$ is the solution of Eq. 13 on $[t_j, t_{j+1}]$ subject to

$$(38) \quad u = 0 \quad \text{on } t = t_j,$$

$$(39) \quad u = (t - t_j)^3 \quad \text{on } x = \pm 1.$$

The condition Eq. 39 is satisfied for

$$u = P_6(x, t - t_j)$$

and hence, by superposition, we also satisfy Eq. 38 if we write

$$(40) \quad Q_j(x, t) = Q(x, t - t_j) = P_6(x, t - t_j) + R(x, t - t_j)$$

where $R(x, t)$ is the solution of Eq. 13 subject to

$$(41) \quad u = 0 \quad \text{on } x = \pm 1$$

$$(42) \quad u = -P_6(x, 0) \quad \text{on } t = 0.$$

Now

$$P_6(x, 0) = -\frac{61}{120} + \frac{5}{8}x^2 - \frac{1}{8}x^4 + \frac{1}{120}x^6$$

and it is not difficult to deduce that

$$(43) \quad R(x, t) = \sum_{k=1}^{\infty} e_k \cos \alpha_k x e^{-\alpha_k^2 t}$$

where

$$\alpha_k = \left(k - \frac{1}{2}\right)\pi$$

and

$$e_k = (-1)^{k-1} 12(\alpha_k)^{-7}$$

The values e_k decrease rapidly with k (being proportional to k^{-7}), and specifically

$$e_1 \simeq 0.5, e_2 \simeq 0.0002, e_3 \simeq 0.000007, \dots$$

Hence very few terms, typically 1, 2 or 3, are required in the expansion Eq. 43, and so the representation Eq. 37 is compact.

Thus we finally obtain a family of particular solutions, corresponding to the individual terms

$$1, t, t^2, t^3, (t - t_1)_+^3, (t - t_2)_+^3, \dots, (t - t_m)_+^3$$

in the spline Eq. 32, namely

$$(44) \quad P_{2i}(x, t) \quad (i = 0, 1, 2, 3); \quad Q(x, t - t_j)_+ \quad (j = 1, \dots, m)$$

where

$$Q(x, t - \lambda)_+ = \begin{cases} Q(x, t - \lambda) & (t \geq \lambda) \\ 0 & (t \leq \lambda) \end{cases}$$

and

$$Q(x, t) = P_6(x, t) + R(x, t)$$

for $R(x, t)$ given by Eq. 43.

We have adopted the family of particular solutions Eq. 44 very successfully in approximation methods for solving a variety of fixed boundary problems for the heat equation, corresponding to boundary conditions of the form

$$u = f(t) \quad \text{on } x = \pm 1.$$

We believe that the family Eq. 44 is appropriate for many Stefan problems in which solutions grow with t , such as the problem considered in § 6.1 below.

4 Approximation Techniques for Boundary Conditions

Once a basis of particular solutions ϕ_j has been determined, the (numerical) solution is expressed in the finite form

$$u \simeq u_n = \sum_{j=1}^n c_j \phi_j$$

The next key requirement is that boundary conditions

$$(45) \quad B_1 u = 0 \quad \text{on } \Gamma$$

should be fitted by some sound criterion, where Γ is initially regarded as a fixed boundary. Assuming that $B_1 u$ is linear in u and its derivatives, the equation (45) must be used to obtain a system of linear equations for the determination of the parameters c_j .

4.1 The Collocation Method

A classical and extremely simple technique to apply is to satisfy Eq. 45 exactly on a set of n suitably chosen collocation points, thus providing a well-determined linear algebraic system. The key questions underlying this are those of selecting collocation points and of establishing convergence. Two alternatives for collocation point selection are now discussed.

4.1.1 Orthogonal Polynomial Zeros

If the particular solutions involve polynomials in one of the variables, and if the region S is bounded between parallel lines, then collocation may be carried out at the zeros of an orthogonal polynomial such as the Chebyshev polynomial T_n . For example, if the polynomials P_{2j}, P_{2j+1} of §3.3 are used to solve the heat equation between $t = 0$ and $t = T$, then collocation points may be chosen as the zeros of $T_n^*(t/T)$.

4.1.2 Basis Function Zeros - Equiangular Points

In a separation of variables process, an infinite expansion is normally obtained. If the particular solutions method adopts the separable variables basis functions, then it is reasonable to regard this method as one which attempts to mimic the partial sum in the true infinite series expansion. A natural collocation procedure is then based on setting to zero the first neglected term in the expansion. For example, in § 2 the approximation Eq. 8 was obtained by collocation at the zeros of

$$J_\alpha(r\sqrt{\lambda}) \cos \alpha\theta$$

for $\alpha = \alpha_{N+1}$, namely the equally angled zeros of $\cos \alpha_{N+1}\theta$, and this led to extremely good results. There are many applications, where there is a (multiplicative) term of form $\cos \alpha\theta$ or $\sin \alpha\theta$ in the separable variables solution, and in such a case the use of equiangular collocation appears to be justifiable and indeed was advocated in [5].

However, these collocation points are based on angles which are independent of the boundary shape, and the possibility has always been present that for certain types of boundaries the method might fail. It comes, therefore as something of a surprise, but also as a fascinating discovery, to observe as we do in § 6 below that the equiangular collocation method can diverge for a relatively simple elliptic equation in a region exterior to an ellipse, where a least squares method converges. The nature of the divergence appears to be similar to that which sometimes occurs in algebraic polynomial interpolation at equally spaced points on an interval (the Runge Phenomenon), but it is somewhat more surprising, since equally spaced points are generally excellent for interpolation by trigonometric polynomials (ie. sine and cosine functions).

4.2 The Least Squares and Galerkin Methods

A less convenient but generally more robust procedure than collocation is to fit Eq. 45 by least squares over a set of $m(> n)$ discrete points which model the boundary. This leads to an over-determined system of m equations in n unknowns, which are solved in a least squares sense by a standard procedure (such as Givens rotations). Such a method is inevitably more expensive.

An alternative, but somewhat similar, method is the Galerkin method, in which the error (in the boundary condition) is made orthogonal to the chosen set of basic functions. However, this method is not easy to formulate on non-rectangular two-dimensional boundaries.

5 Iterative Techniques for Free Boundaries

In a free boundary problem, it is necessary to determine both the solution u and the position of (part of) the boundary Γ at which two boundary conditions are specified:

$$(46) \quad B_1(u) = 0 \quad \text{on } \Gamma$$

$$(47) \quad B_2(u) = 0 \quad \text{on } \Gamma$$

The general technique is to determine sequences $u^{(k)}, \Gamma^{(k)}$ of approximations to u and Γ , $u^{(k+1)}$ being obtained from Eq. 46 and $\Gamma^{(k+1)}$ being determined from Eq. 47 based on some initial guess $\Gamma^{(0)}$ at the position of Γ . If Γ is fixed in Eq. 46 then a collocation or least squares method §. 4 defines $u^{(k+1)}$. If u is fixed in Eq. 47, then this effectively becomes a nonlinear equation typically expressed in terms of its polar distance r for any given θ or in terms of its distance x for any given time t or distance y . Sometimes this nonlinear equation may be readily solved, as it stands, by a standard numerical method such as Newton iteration, using as initial guess the solution u and free boundary Γ determined already for a smaller value of n . Indeed a damped Newton iteration is used successfully for larger values of u in §. 6 below. However, a simpler technique which, if well chosen, can

be globally convergent, is to write the condition Eq. 47 as an equation with both left and right hand sides, say

$$(48) \quad F(u, \Gamma) = G(u, \Gamma)$$

and then to adopt an iteration of the form

$$(49) \quad F(u^{(k)}, \Gamma^{(k+1)}) = G(u^{(k)}, \Gamma^{(k)})$$

to determine $\Gamma^{(k+1)}$ (at discrete positions). This idea is used very successfully for almost all the results in § 6.1, § 6.2 below.

This part of the formulation of a numerical method is probably the most difficult in practice. There are typically several obvious ways of reforming Eq. 47 as Eq. 48, and a number of the resulting iterations may diverge. There is at present a certain amount of luck involved in determining a good iteration, based on a process of intelligent trial and error. It is also advantageous to start with a reasonable guess at the true position of Γ , and to solve the numerical problem first for a small value of n . Then solutions may be developed progressively and more accurately for a succession of larger values of n . Ideally we wish to establish the convergence of the free boundary iteration, but this appears to be very difficult to achieve in practice.

6 Two Particular Free Boundary Problems

In the context of our overall discussion above, and in order to show what can be achieved, we discuss two applications which were first introduced by us in [6], and indicate ways in which the approaches could be extended.

6.1 A Stefan Problem for the Heat Equation

Suppose that u is the required solution to the following Stefan problem, which has also been discussed by [9].

$$(50) \quad L(u) \equiv u_{xx} - u_t = 0 \quad \text{in } S : 0 \leq t \leq T, \quad 0 \leq x \leq X(t)$$

$$(51) \quad B_0(u) \equiv u_x = 0 \quad \text{on } C : x = 0$$

$$(52) \quad B_1(u) \equiv u - x = 0 \quad \text{on } \Gamma : x = X(t)$$

$$(53) \quad B_2(u) \equiv X'(t) + u_x - 1 = 0 \quad \text{on } \Gamma$$

where C is a fixed boundary (or axis of symmetry) and Γ is a free boundary with initial position

$$(54) \quad X(0) = 0$$

Table 1: Error Estimates for Stefan Problem

n	K_n	$\ B_1(u_n)\ $	$\ u_{n+1} - u_n\ $	$\ X_{n+1} - X_n\ $
6	15	2×10^{-4}	2×10^{-4}	6×10^{-5}
7	9	8×10^{-5}		
8	8	3×10^{-5}	3×10^{-5}	5×10^{-6}
9	8	1×10^{-5}		
10	8	4×10^{-6}	4×10^{-6}	7×10^{-7}

Then, adopting as particular solutions the even polynomials P_{2j} of Eq. 22, we may approximate u by

$$(55) \quad u_n = \sum_{j=1}^n c_j P_{2j}(x, t)$$

and represent Γ by the approximation

$$(56) \quad \Gamma_n : X_n(t) = \sum_{j=1}^n d_j t^j$$

Boundary conditions are now solved by a two-stage iterative process (for $k=0,1,2,\dots$):

(i) Determine $\{c_j\}$ in $u_n^{(k)}$ by collocation to Eq. 52 at the zeros of $T_n^*(t/T)$

(ii) Determine $\{d_j\}$ in $X_n^{(k)}$ by solving

$$(57) \quad [X_n^{(k+1)}]' = 1 - \frac{\partial u_n^{(k)}}{\partial x}$$

at the zeros of $T_n^*(t/T)$ on $X_n^{(k)}$ where T_n^* is the shifted Chebyshev polynomial of degree n .

The process works well in practice with initial approximations

$$(58) \quad X_6^{(0)}(t) = t; \quad X_n^{(0)}(t) = X_{n-1}(t) \quad (n > 6)$$

where $X_n(t)$ denotes the limit of the sequence $\{X_n^{(k)}(t)\}$ and $u_n(t)$ denotes the limit of the sequence $\{u_n^{(k)}(t)\}$.

The Step (i) is based on orthogonal (Chebyshev) collocation, as discussed in §. 4.1, and step (ii) adopts an iteration of type Eq. 49 discussed in §. 5.

In Table 1 are given the maximum absolute values of $B_1(u_n)$, $u_{n+1} - u_n$, and $X_{n+1} - X_n$ over discrete point sets in steps of 0.1 in x and t , for $T = 1$. From these results we estimate that Γ and u have been determined correctly to 6 and 5 decimal places, respectively, at all points of S with just $n = 10$ parameters for each. The number of iterations needed for each n is also shown.

One improvement that we propose to this method is to write $X_n(t)$ in the form

$$(59) \quad X_n(t) = \sum_{j=0}^n d_j T_j^*(t/T)$$

so that

$$(60) \quad X'_n(t) = \frac{2}{T} \sum_{j=1}^n d_j j U_{j-1}^*(t/T)$$

Then, if we change the collocation points to the n zeros of $U_n^*(t/T)$, Eq. 57 becomes a process of collocating a (2nd kind) Chebyshev polynomial at (2nd kind) Chebyshev zeros, which can be carried out extremely rapidly by a discrete Fourier transform.

As a second improvement, or extension, in the method, we propose that a large range $[0, T]$ of t should be dealt with by using a piecewise approximation method, and for this purpose we believe that the piecewise particular solutions procedure derived in § 3.4 would prove highly effective. A different set of collocation points in t would be required in this case and equally spaced abscissae are proposed, since they generally work well for splines.

6.2 An Interface Problem for Laplace's Equation

The potential ϕ and stream function ψ of a perfect fluid satisfy the Cauchy-Riemann equations

$$(61) \quad \phi_x = \psi_y, \quad \phi_y = -\psi_x$$

and hence correspond to the real and imaginary parts of an (analytic) "complex potential"

$$(62) \quad u(x, y) = \phi(x, y) + i\psi(x, y).$$

Consider such a flow in the region of Figure 2, subject to the boundary conditions shown, and note that $z^{1/2}$ -type singularities occur at D and E and that B is a stagnation point.

A preliminary transformation

$$(63) \quad z_{new} = c - z^{1/2} \quad (z = x + iy)$$

where $c = \sqrt{a}$, $a = DE$, $b = CD$, removes the singularity at D and gives the region of Figure 3.

Equations Eq. 61 still apply, and boundary conditions become

$$(64) \quad B_0(u) : \begin{cases} \psi = 1 & \text{on } y = 0 \quad (x > 0) \\ \phi = 0 & \text{on } y = 0 \quad (x < 0) \end{cases}$$

$$(65) \quad B_1(u) : \begin{cases} \phi = -2 & \text{on } x = c & (DC) \\ \psi = 0 & \text{on } (x - c)^2 - y^2 + b = 0 & (CB) \end{cases}$$

$$(66) \quad B_2(u) : \quad \psi = 0 \quad \text{on } \Gamma \quad (AB)$$

$$(67) \quad B_3(u) : \quad \phi - 2(x - c)y = 0 \quad \text{on } \Gamma \quad (AB)$$

The condition $B_3(u)$ corresponds to the condition $\phi + y = 0$ in Figure 2.

A remarkable economy and accuracy is achieved by using the approximation

$$(68) \quad u \simeq u_n = i + \sum_{j=1}^n c_j z^{j-1/2},$$

which corresponds to

$$(69) \quad \phi \simeq \phi_n = \sum_{j=1}^n c_j r^{j-1/2} \cos(j-1/2)\theta$$

$$(70) \quad \psi \simeq \psi_n = 1 + \sum_{j=1}^n c_j r^{j-1/2} \sin(j-1/2)\theta$$

Note that Eq. 69 Eq. 70 automatically satisfy $B_0(u)$ and remove the singularity at E.

A collocation process is based on n equally spaced lines.

$$(71) \quad \theta = \theta_j = 2j\pi/(n+1), \quad (j = 1, \dots, n)$$

namely the zeros of $\sin(n+1/2)\theta$ (as proposed in §4.1).

The free boundary Γ is now represented in the discrete form

$$(72) \quad \Gamma_n : \quad r = r(\theta) \quad \text{at } \theta = \theta_j \quad (j = n-p+1, \dots, n)$$

where the latter values θ_j are those lines Eq. 71 which intersect Γ_n . The fixed and free boundary conditions Eq. 65 Eq. 66 Eq. 67 are then satisfied by the iterative process:

(i) Determine $u_n^{(k+1)}$ by imposing B_1 and B_2 at the n positions Eq. 71 on DC, CB, $\Gamma_n^{(k)}$

(ii) For $\theta = \theta_j$ ($j \geq n-p+1$), determine $r^{(k+1)}(\theta)$ on $\Gamma_n^{(k+1)}$ by solving

$$(73) \quad \phi_n^{(k)}(r^{(k)}, \theta) = 2(r^{(k+1)} \cos \theta - c) r^{(k+1)} \sin \theta.$$

The condition (i) gives n simultaneous equations for c_j in $u_n^{(k+1)}$, while (ii) gives a quadratic equation, based on an iteration of the type Eq. 49 discussed above, which is solved for each θ for that root $r^{(k+1)}$ nearest to $r^{(k)}$.

The iterative method works very successfully for the case $a = 1.082$, $b = 0.489$ considered by [3], taking as $\Gamma_n^{(0)}$ the transform Eq. 63 of an ellipse with axis $CA = 3.262$ and $CB = 1.8$ in Figure 2. Rapid convergence occurs for $n = 8, 10, 12$, although a damped Newton method was needed to ensure convergence for $n = 14$. All coefficients c_j were observed to be individually converging as $n \rightarrow \infty$.

For $n = 14$, ϕ, ψ, Γ were determined in [6] with an accuracy varying between about 2 decimal places near B, C and about 4 decimal places near D, E, A , a comparable result to that of Charmonman [3] who used hundred of grid points. For $n = 14$, there were $p = 9$ collocation points on Γ_{14} , and so, to tidy up the representation, a cubic spline with 11 parameters

$$(74) \quad \Gamma_{14}^* : s = d_1 + d_2\alpha + d_3\alpha^2 + \sum_{j=1}^8 d_{j+3}(\alpha - \alpha_{j+1})_+^3$$

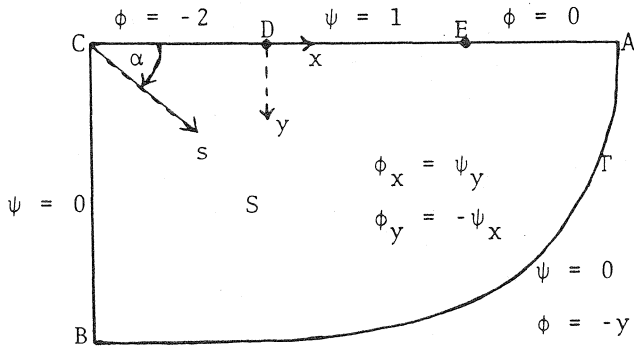


Fig. 2. Charmonman's problem: original region.

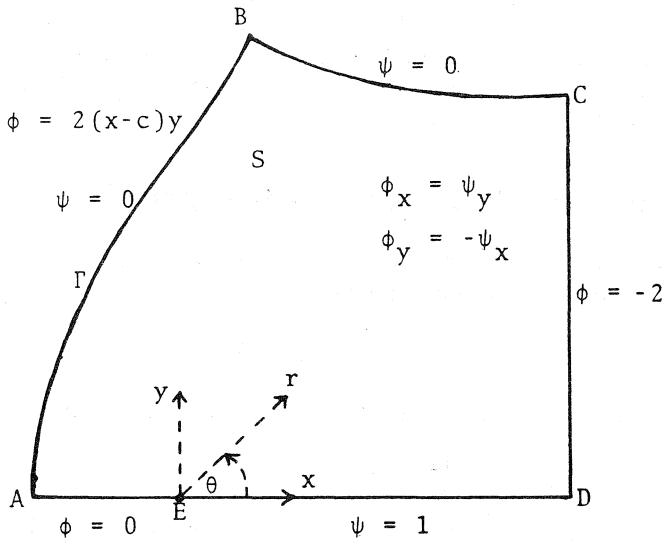


Fig. 3. Charmonman's problem: transformed region.

Table 2: Charmonman's Problem: Final Representations

Coeffs. of u_{14}		Coeffs. of Γ_{14}^*	
c_1	-2.09609×10^0	d_1	3.26221×10^0
c_2	2.95177×10^{-1}	d_2	-4.01475×10^0
c_3	-1.44368×10^{-1}	d_3	1.27836×10^0
c_4	-2.62067×10^{-2}	d_4	1.67279×10^0
c_5	2.18361×10^{-2}	d_5	9.80398×10^{-1}
c_6	-9.51682×10^{-3}	d_6	5.34046×10^{-1}
c_7	-1.34656×10^{-3}	d_7	-3.11432×10^{-2}
c_8	2.58528×10^{-3}	d_8	-1.07110×10^0
c_9	-2.53178×10^{-3}	d_9	-1.06654×10^0
c_{10}	6.43614×10^{-4}	d_{10}	-2.07028×10^0
c_{11}	3.08907×10^{-4}	d_{11}	-1.51789×10^0
c_{12}	-5.62240×10^{-4}		
c_{13}	2.53651×10^{-4}		
c_{14}	-1.07529×10^{-4}		

was fitted to Γ_{14} in Figure 2 in (s, α) coordinates. The parameters d_j were determined by collocation to Γ_{14} at $\alpha = \alpha_1, \alpha_2, \dots, \alpha_9$ corresponding to $\theta = \theta_n, \theta_{n-1}, \dots, \theta_{n-8}$ in Figure 3, subject to the constraints that Γ_{14}^* should meet CB and EA at right angles. The resulting parameters $\{c_j\}$ and $\{d_j\}$ in Eq. 68 Eq. 74 are given in Table 2.

We note that this method has been remarkably effective and accurate. However, we believe that increased accuracy and reliability would be achieved by adopting a least squares rather than a collocation method. Effectively, more than n collocation points/angles would be chosen in the method above, to ensure sufficiently dense coverage of the boundaries, and this would lead to an overdetermined system of linear equations (solved in a least squares sense) for $\{c_j\}$ in part (i) of the iterative process.

7 Preliminary work on a bush-fire problem

If we model an area of bush as a self-heating reactive medium, then conservation of energy leads to the reaction-convection-diffusion equation

$$(75) \quad \frac{\partial u}{\partial t} + \underline{w} \cdot \nabla u = \nabla^2 u + f(u)$$

(See for example [2].) For co-moving coordinates sitting at the reaction front,

$$(76) \quad \frac{\partial u}{\partial t} + \underline{v} \cdot \nabla u = 0$$

where \underline{v} is the velocity vector of the reaction wave. Considering the preheated region ahead of the wave, where $f(u)$ can be linearised, Eq. 75, Eq. 76 combine to give

$$(77) \quad \underline{W} \cdot \nabla u = \nabla^2 u + f'(u_0) \cdot (u - u_0)$$

where $\underline{W} = \underline{w} - \underline{v}$, and u_0 is an equilibrium solution of Eq. 75 (i.e. $f(u_0) = 0$). This is an equation for the "outer" solution in the regular perturbation procedure. In two dimensions x, y , assuming that wind speed is much greater than the speed of the reaction wave, we may take the components of \underline{W} to be

$$(78) \quad W_x = w, \quad W_y = 0$$

and Eq. 77 then becomes

$$(79) \quad w \frac{\partial u}{\partial x} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + f'(u_0) \cdot (u - u_0)$$

Let $V = u - u_0$, so that $V(0) = 0$, and then

$$(80) \quad \frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} = w \frac{\partial V}{\partial x} - \alpha V$$

where $\alpha = f'(0)$. In the case $\alpha = 0$, the equation also arises in soil physics ([7]). If we further write

$$(81) \quad V = e^{\frac{1}{2}wr \cos \theta} \phi$$

then it follows from Eq. 80, Eq. 81 that

$$(82) \quad \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = \left(\frac{w_1}{2}\right)^2 \phi$$

where

$$(83) \quad w_1 = \sqrt{w^2 - 4\alpha}$$

A solution of Eq. 79 is sought, in a region exterior to some unknown closed curve Γ , which decreases to an ambient value (of zero, say) as $x^2 + y^2 \rightarrow \infty$. By separation of variables, we obtain the infinite expansion

$$(84) \quad u(r, \theta) = u_0 + e^{\frac{1}{2}wr \cos \theta} \sum_{j=1}^{\infty} c_j K_{j-1} \left(\frac{1}{2}w_1 r\right) \cos(j-1)\theta$$

where K_j is the modified Bessel function of order j and where, for simplicity, we assume solutions (and boundary conditions) that are even in θ (to eliminate sine terms).

To complete the problem specifications, two appropriate boundary conditions are imposed on Γ , and u and Γ are to be determined iteratively.

7.1 Fixed Boundary Problem

A prerequisite, in order to later attempt to solve a free boundary problem, is to be able to solve a fixed boundary problem, namely Eq. 79 subject to

$$(85) \quad u = A \quad \text{on } \Gamma,$$

where Γ is fixed and A is a constant. The method should be robust over a variety of such boundary shapes Γ . For simplicity we restrict discussion to the case $u_0 = 0$, $\alpha = 0$, $w = w_1 = 4$.

In fact this problem is quite challenging, and we have needed to adopt a least squares algorithm only after first experiencing an unexpectedly unreliable collocation procedure. Following the discussion of §3 and observing the form of Eq. 84 we are immediately led to the exterior approximation

$$(86) \quad u_n = e^{\frac{1}{2}wr \cos \theta} \sum_{j=1}^n c_j K_{j-1} \left(\frac{1}{2} w_1 r \right) \cos(j-1)\theta$$

where c_j are undetermined parameters. In practice, to avoid overflow in the functions K_{j-1} , it is preferable to replace c_j and K_{j-1} , respectively by the scaled values

$$(87) \quad c_j^* = 2^j j! c_j, \quad K_{j-1}^* = 2^{-j} (j!)^{-1} K_{j-1}$$

7.2 Collocation Procedure

Since Γ is symmetrical about $\theta = 0$ (by our assumption of an even solution), it is natural to propose collocating Eq. 85 at the n positive zeros of $\cos n\theta$, namely

$$(88) \quad \theta = \left(k - \frac{1}{2}\right)\pi/n, \quad (k = 1, 2, \dots, n)$$

This leads to n simultaneous equations for c_j .

We tested this procedure, with $A = 1.2$ in Eq. 85, for a variety of boundaries, and specifically:

- (i) Circle: $r = 1$
- (ii) Ellipse: $r = 0.4875(1 - 0.625 \cos \theta)^{-1}$
- (iii) Quasi-ellipse: $r = 0.8 + 0.5 \cos \theta$

The results for the circle were excellent, with u correct to about 4 significant figures for $n = 5$, and are shown in Table 3. However, surprising results were obtained for both the ellipse and the quasi-ellipse.

Results for the ellipse with $n = 10$ are shown in Table 4, and it will be noted that, although the approximations u_n are converging for small θ , they are diverging, and indeed oscillating wildly, for a large range of θ . Results for the quasi-ellipse were also inaccurate in a range around $\theta = \pi$ and indeed appeared to be diverging.

Table 3: Collocation on $\Gamma : r = 1$ at $\theta = (2k - 1)\pi/10$.
Print of Boundary Approximation at $\theta = l\pi/32$ ($n = 5$)

j	c_j^*	l	u_5	l	u_5
1	3.60853	0	1.2015	20	1.1996
2	-4.50695	4	1.1995	24	1.2003
3	0.80203	8	1.1992	28	1.2001
4	-0.11987	12	1.2008	32	1.1997
5	0.01414	16	1.2000		

Table 4: Collocation on $\Gamma : r = .4875(1 - .625 \cos \theta)^{-1}$ at $\theta = (2k - 1)\pi/20$.
Print of Boundary Approximation at $\theta = l\pi/20$ ($n = 10$)

j	c_j^*	l	u_5	l	u_5
1	1.23525×10^0	0	1.2020	10	1.0039
2	4.20454×10^{-3}	1	1.2000	11	1.2000
3	-3.89014×10^{-2}	2	1.1975	12	1.7910
4	-2.28849×10^{-2}	3	1.2000	13	1.2000
5	-1.40183×10^{-2}	4	1.2052	14	-0.2365
6	-9.26773×10^{-3}	5	1.2000	15	1.2000
7	-6.40033×10^{-3}	6	1.1844	16	3.9359
8	-4.26193×10^{-3}	7	1.2000	17	1.2000
9	-2.28635×10^{-3}	8	1.2560	18	-2.8369
10	-6.68032×10^{-4}	9	1.2000	19	1.2000
				20	5.7971

The results confirm a new divergence phenomenon for equi-spaced (in angle) collocation of a separable variable expansion involving trigonometric polynomials, analogous to the well-known Runge phenomenon for equi-spaced (in distance) collocation of an algebraic polynomial.

7.3 Least Squares Procedure

Fortunately the use of a least squares method, in the fitting of Eq 85 at $m > n$ selected angles θ on Γ , is robust and does not display the oscillating behaviour of the collocation method. Results for the ellipse ((iii) above for $n = 10$, for which collocation failed, are given in Table 5, and the nearly 3 significant figures obtained are very satisfactory. Indeed this procedure has been found to be reliable for a wide variety of boundaries.

Table 5: Least Squares on Γ : $r = .4875(1 - .625 \cos \theta)^{-1}$ at $\theta = k\pi/20$.
 Print of Boundary Approximation at $\theta = l\pi/20$ ($n = 10$)

j	c_j^*	l	u_5	l	u_5
1	1.23488×10^0	0	1.2094	10	1.2031
2	3.50674×10^{-3}	1	1.2051	11	1.2025
3	-3.87196×10^{-2}	2	1.1958	12	1.1967
4	-2.12595×10^{-2}	3	1.1895	13	1.1995
5	-1.07538×10^{-2}	4	1.1919	14	1.2031
6	-4.81738×10^{-3}	5	1.2010	15	1.1983
7	-1.75446×10^{-3}	6	1.2076	16	1.1986
8	-4.71689×10^{-4}	7	1.2040	17	1.2027
9	-8.18185×10^{-5}	8	1.1959	18	1.1989
10	-6.78626×10^{-6}	9	1.1961	19	1.1983
				20	1.2015

7.4 Free Boundary Problems

In order to tackle a problem for Eq. 79 in which Γ is a free boundary, it is necessary to formulate a physically appropriate pair of boundary conditions on Γ , and thence to solve the exterior problem iteratively. From §7.2, we advocate the use of a least squares procedure of boundary approximation. However, success will depend on the choice of the right iteration procedure and of a good enough initial estimate for Γ .

These observations are relevant to other studies of fire state, which we sometimes based on elliptical boundary models (e.g. [1]). A discussion of other wild fire models is given in [8].

8 Conclusions

We have drawn the readers' attention to a particular solutions method which, although based on classical analytical techniques (such as separation of variables), is not too often exposed in the literature. Although applications are limited to relatively simple model equations, spectacular successes have been achieved for some difficult and relevant problems.

Attention has also been given to the various details which need to be considered when formulating a particular solutions method. In particular, although equi-spaced collocation can prove very convenient, we have reported a (specific) boundary value problem in which a natural equi-angled collocation procedure can lead to divergence (akin to the Runge phenomenon).

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