An iterative analytic series method for Laplacian problems with free and mixed boundary conditions

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Abstract

Mixed boundary value problems occur in a wide variety of applications in applied mathematics. These problems are characterised by a combination of Dirichlet and Neumann conditions along at least one boundary. For example, problems in both saturated and unsaturated flow usually contain mixed boundary conditions. Historically, only a small subset of these problems could be solved using analytic series methods, by using an appropriate coordinate transformation or choice of axes.

However, there are some striking similarities between the mixed boundary problem and the free boundary problem, where the location of one boundary is initially unknown. This unknown boundary is subject to two boundary conditions, and so the problem can be fully defined. In this paper, I will point out the similarities between mixed boundary and free boundary problems. I will consider mixed boundary conditions of the form

$$\alpha(x,y)\phi(x,y) + \beta(x,y)\frac{\partial}{\partial m}\phi(x,y) = \gamma(x,y),$$

where ϕ satisfies Laplace's equation. Finally, I will present an iterative method to find analytic series solutions for problems of this type.

Contents

1 Introduction

Laplacian boundary value problems occur in a wide range of engineering and applied mathematics applications. Problems encountered in these areas range from straightforward Dirichlet or Neumann type problems through mixed Dirichlet-Neumann type problems to the much more difficult free boundary problems. For example, problems of these types regularly occur in the study of transport processes in porous media. In particular, infiltration and seepage problems generally involve either mixed and/or unknown boundary value problems. In most practical applications, the boundary geometries are irregular, and in the past purely numerical schemes were usually chosen to obtain an approximate solution.

Recently, analytic series solutions have been developed to solve both known and unknown boundary problems, on irregular solution domains [1, 2, 4]. The series used in the solution is obtained using the classic method of separation of variables. These methods have several advantages over their numerical counterparts. They are fast and accurate, with exact global **maximum** error bounds available. The solution is continuous throughout the flow field, and can be used to drive numerical advection-diffusion solvers, without recalculating the flow field at each mesh refinement step. In addition, all the associated parameters are immediately available, including the stream function and velocity field.

Another advantage of the series approach is that the solution process does not depend on the method used to represent the boundary geometries. As a consequence, cubic splines and other commonly available interpolants can be used for discrete boundary data, as well as exact formulations for known geometries. In particular, for free boundary problems the free boundary location can be approximated using cubic splines, or any other interpolants, and the knot spacing can be changed arbitrarily during the solution process.

Classically, series methods have only been applicable to simple mixed boundary condition problems defined on regular boundaries, when the coordinate axes can be chosen to align with the boundaries, and (apart from some straightforward exceptions) each boundary condition is exclusively either Dirichlet or Neumann. Analytic series methods have been extended to irregular boundary geometries and free boundary problems, but the solution has not been directly applied to the general mixed boundary value problem. Although free boundary problems implicitly contain a mixed boundary value problem, the solution method entails solving a sequence of known boundary value problems. On each of these boundaries (including the free boundary), the boundary conditions are either Dirichlet or Neumann, but not both.

In this paper, I compare mixed boundary and free boundary problems, and provide an iterative method to solve the classical mixed boundary value problem. The method will be used to provide solutions for a saturated seepage problem. At the algorithmic level, there is a striking similarity between the solution techniques for the two types of problem. These similarities will be discussed, and I will indicate the advantages to solving mixed boundary problems that flow on from these similarities.

2 Problem Definition

In this section, the general Laplacian mixed boundary value problem is defined. In the interior of the solution domain, Laplace's equation for $\phi(x, y)$

is satisfied:

$$\nabla^2\phi = \frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} = 0. \tag{1}$$

On (at least) one boundary, a boundary condition of the following form must be satisfied:

$$\alpha(x,y)\phi(x,y) + \beta(x,y)\frac{\partial}{\partial m}\phi(x,y) = \gamma(x,y), \tag{2}$$

where $\frac{\partial}{\partial m}$ denotes differentiation normal to the boundary. We assume that this boundary condition holds on the boundary $y = f(x)$, and can't be broken down into separate Dirichlet and Neumann conditions by a suitable choice of axes or coordinate transformation. The mixed boundary condition along $f(x)$ becomes:

$$\bar{\alpha}(x)\bar{\phi}(x) + \bar{\beta}(x)\frac{\partial}{\partial m}\bar{\phi} = \bar{\gamma}(x) \tag{3}$$

where

$$\bar{\phi}(x) = \phi(x, f(x)), \quad \frac{\partial}{\partial m}\bar{\phi}(x) = \frac{\partial}{\partial m}\phi(x, f(x)) \tag{4}$$

and

$$\bar{\alpha}(x) = \alpha(x, f(x)), \quad \bar{\beta}(x) = \beta(x, f(x)), \quad \bar{\gamma}(x) = \gamma(x, f(x)) \tag{5}$$

There are three different categories that the mixed boundary condition described by equation (1) can be broken into. They are:

1. $\bar{\alpha}(x)$, $\bar{\beta}(x)$ are constant functions of x;

2. $\bar{\alpha}(x)$, $\bar{\beta}(x)$ are continuous functions of x;

3. $\bar{\alpha}(x)$, $\bar{\beta}(x)$ are discontinuous functions of x.
   For example, $\bar{\phi}(x)$ is specified on $[0, a)$ and $\frac{\partial}{\partial m}\bar{\phi}(x)$ is specified on $[a, s]$.

Problems that fall into the first category are readily solved using existing methods. For problems in the second category, the solution method is not as straightforward as in the first case, but these problems can still be solved reasonable easily. The third category of problems are the most difficult, and it is to problems of this type that the rest of this paper will be devoted.

2.1 A Specific Problem

In order to develop the solution method, we will focus on a specific problem. A rectangular boundary geometry has been chosen, so that the focus is on the mixed boundary condition, rather than the solution domain. Note that the method described in this paper is readily applied to an arbitrary boundary geometry.

Consider steady saturated seepage from a dam through an aquifer to a pond. The surface of the aquifer between the base of the dam wall and the pond is horizontal, and the aquifer of length s and constant depth 1 lies on top of a horizontal impermeable aquiclude. Upstream, water has ponded to a height h_2, while downstream the ponded water has height h_1

($h_1 < h_2$). Along the upstream section of the soil surface, the discharge rate is known, while the downstream section acts as a seepage face. Figure 1 gives a schematic of the soil horizon.

Mathematically, the problem can be formulated as follows. Inside the saturated soil, seepage is governed by Darcy's law. Assuming constant hydraulic conductivity K and invoking the continuity condition, the hydraulic potential ϕ is governed by Laplace's equation, inside the aquifer:

$$\nabla^2\phi(x,y) = 0. \tag{6}$$

Along the vertical boundaries at $x = 0$ and $x = s$, the boundary conditions are given by

$$\phi(0,y) = h_1, \qquad \phi(s,y) = h_2. \tag{7}$$

Along the impermeable aquiclude $y = 0$, the boundary condition becomes

$$K\frac{\partial}{\partial y}\phi(x,0) = 0. \tag{8}$$

Along the soil surface $y = 1$, the mixed boundary condition is

$$\phi(x,1) = 1, \qquad 0 \le x < a; \tag{9}$$

$$K\frac{\partial}{\partial y}\phi(x,1) = R(x), \qquad a \le x \le s. \tag{10}$$

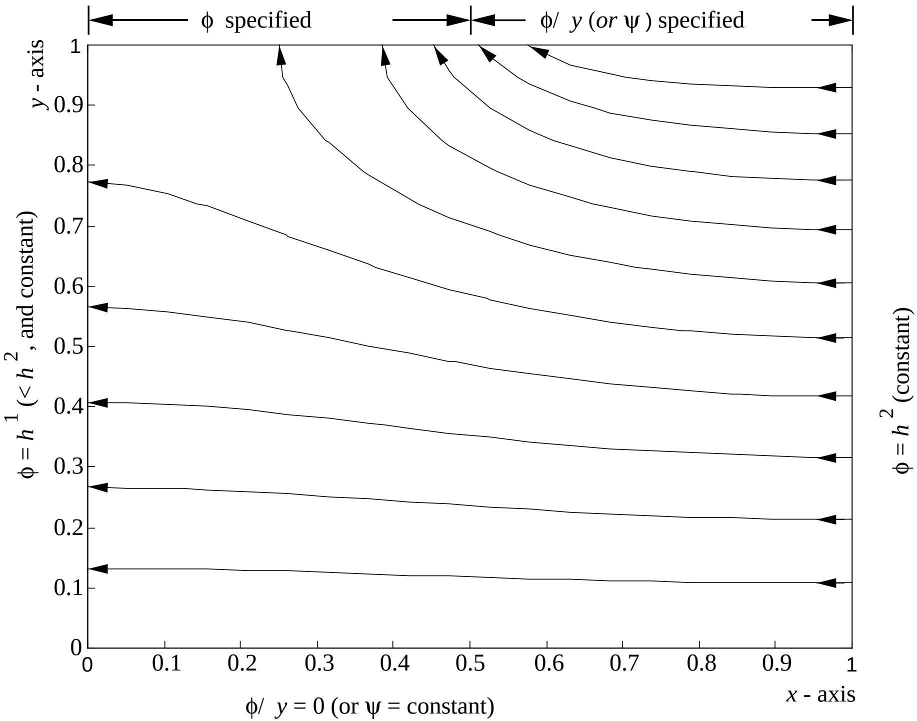

Figure 1: Schematic of the saturated flow domain.

3 Series Solution

The problem formulated in the previous section needs to be transformed slightly [3], so that separation of variables can be used to obtain an analytic series solution. Letting

$$\phi(x,y) = h_1 + \frac{x(h_2 - h_1)}{s} + \varphi, \tag{11}$$

then φ satisfies Laplace's equation:

$$\nabla^2 \varphi = 0 \tag{12}$$

with homogeneous side boundary conditions

$$\varphi(0,y) = 0, \qquad \varphi(s,y) = 0 \tag{13}$$

and homogeneous bottom boundary condition

$$\frac{\partial}{\partial y}\varphi(x,0) = 0. \tag{14}$$

The classical method of separation of variables can now be applied to (12). Using the homogeneous side (13) and bottom (14) boundary conditions, the analytic series solution is readily shown to be

$$\varphi(x,y) = \sum_{n=1}^{\infty} A_n \cosh\left(\frac{n\pi y}{s}\right) \sin\left(\frac{n\pi x}{s}\right). \tag{15}$$

The series solution for the original problem becomes

$$\phi(x,y) = h_1 + \frac{x(h_2-h_1)}{s} + \sum_{n=1}^{\infty} A_n \cosh\left(\frac{n\pi y}{s}\right)\sin\left(\frac{n\pi x}{s}\right). \qquad (16)$$

Note that this series solution satisfies both the inhomogeneous side boundary conditions (7) and homogeneous bottom boundary condition (8) of the original problem exactly. The top boundary condition (9), (10) is used to evaluate the series coefficients A_n, and so fully define the solution. Unfortunately, the classical approach breaks down at this point, as the boundary condition is not a linear combination of ϕ and $\frac{\partial\phi}{\partial y}$. Consequently, the orthogonality relationship cannot be used (directly!) to determine the A_n.

4 Free Boundary Problems

The mixed boundary problem defined and discussed in the previous sections is a steady, *saturated* flow problem. Unsaturated seepage problems occur when there is not enough water available to completely saturate the aquifer. For example, in hillside seepage the water lies below the soil surface when the recharge rate is not high enough to ensure saturation. Locating the water table location $\eta(x)$ is a free boundary problem. Assuming the water table intersects the soil surface $f(x)$ at some point $x = a$ say, the soil surface and the water table delineate the saturated aquifer boundary. Letting this boundary be denoted by $y^t(x)$, then

$$y^t(x) = \begin{cases} f(x), & 0 \le x < a \\ \eta(x), & a \le x \le s \end{cases} . \tag{17}$$

The boundary conditions along $y^t(x)$ becomes

$$\phi(x, y^t(x)) = y^t(x), \quad 0 \le x \le s, \tag{18}$$

$$K \frac{\partial}{\partial m} \phi(x, y^t(x)) = R(x), \quad a \le x \le s. \tag{19}$$

The method used [1, 2, 4] to solve for $\eta(x)$ consists of two steps. First, $\eta(x)$ is approximated using splines or some other interpolants. Next, an initial guess of the water table location is made, and then iteratively improved. At each step, $y^t(x)$ is known, and the Neumann condition is used as a cost function to perform the updates. The cost function to be minimised in the L_2 (or least squares) norm sense is

$$C(x) = \left[\int_a^s \left(R(x) - K \frac{\partial}{\partial m} \phi(x, y^t(x)) \right)^2 dx \right]^{\frac{1}{2}} . \tag{20}$$

In essence, the free boundary problem has been reduced to solving a sequence of known boundary value problems. The potential condition (18) is used as the top boundary condition, and thus the implicit mixed boundary problem has been avoided.

4.1 The Free Boundary Condition

The Neumann condition along the water table can be linearised, by using the stream function. The Cauchy Riemann equations for the conjugate stream function $\psi(x, y)$ are given by

$$\frac{\partial \phi}{\partial x} = \frac{\partial \psi}{\partial y}, \qquad \frac{\partial \phi}{\partial y} = -\frac{\partial \psi}{\partial x}. \tag{21}$$

Along $y = \eta(x)$, equation (19) becomes

$$\begin{aligned}
K\frac{\partial}{\partial m}\phi(x, \eta(x)) &= K\left(\frac{\partial}{\partial y}\phi(x, \eta(x) - \frac{\partial}{\partial x}\phi(x, \eta(x))\frac{d}{dx}\eta(x)\right) && (22)\\
&= -K\left(\frac{\partial}{\partial x}\psi(x, \eta(x)) + \frac{\partial}{\partial y}\psi(x, \eta(x))\frac{d}{dx}\eta(x)\right) && (23)\\
&= -K\frac{d}{dx}\bar{\psi}(x) && (24)\\
&= R(x) && (25)
\end{aligned}$$

where $\bar{\psi}(x) = \psi(x, \eta(x))$. Integrating with respect to x, the stream function condition along the free surface becomes

$$\bar{\psi}(x) = r(x), \tag{26}$$

where

$$Kr(x) = -\int R(x)\, dx. \tag{27}$$

With these changes, the cost function (20) to be minimised becomes

$$C(x) = \left[\int_a^s \left(r(x) - \bar{\psi}(x)\right)^2 \, dx\right]^{\frac{1}{2}} . \tag{28}$$

The free surface boundary $\eta(x)$ can be approximated using an almost arbitrary range of interpolants. In this paper, cubic splines are used, as they are universally available and are efficient to use and implement. The cost function can now be evaluated and minimised, now that $\eta(x)$ has been approximated. As the approximation depends on the iteration number, let the approximate water table location at iteration i be denoted by $\eta^{(i)}(x)$.

A wide range of sophisticated methods have been tried by the author and others to minimise the cost function. However, in practice a very simple approach appears to work best. Letting bracketed superscripts indicate the iterate number, the update at each knot point $(\xi_j,\ \eta_j^{(i)})$, $j = 1, \ldots, M$ is based on the following quasi-Newton method:

$$\eta_j^{(i+1)} = \eta_j^{(i)} - C\left(r(x) - \bar{\psi}(x)\right), \tag{29}$$

where C is the quasi-Newton constant. After each iteration, the error in the cost function (28) can be calculated and compared with the previous value.

The continuous nature of the solution allows enormous flexibility when setting up the iterative scheme. In practice, the stability and efficiency of the iterative scheme can be markedly improved, by averaging the point update $\eta_j^{(i+1)}$ at each knot point $(\xi_j,\ \eta_j^{(i)})$ over the interval $[\xi_j - \delta_j, \xi_j + \delta_j]$, where

δ_j is chosen (as small or large as necessary) to enhance the convergence properties. The point estimates $\eta_j^{(i+1)}$ in equation (29) are replaced by the averaged estimates $\hat{\eta}_j^{i+1}$ [1, 5]:

$$\hat{\eta}_j^{(i+1)} = \frac{1}{2\delta_j} \int_{\xi_j - \delta_j}^{\xi_j + \delta_j} \eta^{(i)}(x) - C\left(r(x) - \bar{\psi}(x)\right)\, dx. \tag{30}$$

5 An iterative Method for Mixed Boundary Conditions

For the free boundary problem, the boundary conditions (18), (19) along the upper (soil) surface $y^t(x)$ can be represented as

$$f(x) \text{ known}, \quad 0 \le x < a \quad ; \qquad \eta(x) \text{ unknown}, \quad a \le x \le s; \tag{31}$$

$$\bar{\phi}(x) \text{ known}, \quad 0 \le x < a \quad ; \qquad \bar{\phi}(x) \text{ known}, \quad a \le x \le s; \tag{32}$$

$$\frac{\partial \bar{\phi}}{\partial y} \text{ unknown}, \quad 0 \le x < a \quad ; \qquad \frac{\partial \bar{\phi}}{\partial y} \text{ known}, \quad a \le x \le s. \tag{33}$$

Similarly, the mixed boundary conditions (9), (10) along the soil surface $f(x) = 1$ can be represented as

$$f(x) \text{ known}, \quad 0 \le x < a \quad ; \qquad f(x) \text{ known}, \quad a \le x \le s; \tag{34}$$

$$\bar{\phi}(x) \text{ known}, \quad 0 \le x < a \quad ; \qquad \bar{\phi}(x) \text{ unknown}, \quad a \le x \le s; \tag{35}$$

$$\frac{\partial \bar{\phi}}{\partial y} \text{ unknown}, \quad 0 \le x < a \quad ; \qquad \frac{\partial \bar{\phi}}{\partial y} \text{ known}, \quad a \le x \le s. \tag{36}$$

An inspection of the preceding summaries of the the free and mixed boundary problems reveals a number of similarities. The only significant difference is that $\eta(x)$, $a \le x \le s$ is unknown in the free boundary problem, while $\bar{\phi}(x)$, $a \le x \le s$ is unknown in the mixed boundary problem. In effect, the roles of $\eta(x)$ and $\bar{\phi}(x)$ have been interchanged. This suggests the following iterative approach to solve the mixed boundary problem.

First, approximate $\bar{\phi}(x)$ on the unknown region, from $a \le x \le s$, using cubic splines. Denote this approximation at iteration i by $\bar{\phi}^{(i)}(x)$. Now that the potential is "known" along the entire upper boundary, the series coefficients can be evaluated using the orthogonality relationship. Next, convert the Neumann condition (10) to a stream function condition, so that

$$\bar{\psi}(x) = r(x), \tag{37}$$

on $y = 1$ from $x = a$ to $x = s$.

Finally, make an initial estimate $\bar{\phi}^{(0)}(x)$ of $\bar{\phi}(x)$, $a \le x \le s$ and iteratively improve the estimates using a quasi Newton scheme. Thus, at iteration i, the updated potential at knot $(\xi_j, 1)$, $j = 1, \dots, M$ is given by

$$\bar{\phi}_j^{(i+1)} = \bar{\phi}_j^{(i)} - C\left(r(x) - \bar{\psi}(x)\right), \tag{38}$$

where C is the quasi Newton constant. As for the free boundary problem, these point estimates are replaced by the averaged estimates

$$\hat{\phi}_j^{(i)} = \frac{1}{2\delta_j} \int_{\xi_j-\delta_j}^{\xi_j+\delta_j} \bar{\phi}^{(i)}(x) - C\left(r(x) - \bar{\psi}(x)\right)\, dx. \tag{39}$$

6 Implementation and Solutions

Implementing the series solution first requires that the interpolants for the unknown potential be specified. For the example given in this paper, the Matlab routine `spline` was used. The derivative endpoint conditions for this routine are the 'not a knot' conditions. At the first and last knot points $(a, 1)$ and $(s, 1)$, the potential does not change. So, at any iteration i,

$$\bar{\phi}^{(i)}(a) = h_1, \qquad \bar{\phi}^{(i)}(s) = h_2. \tag{40}$$

Initially, two spline segments were used to approximate the potential from $x = a$ to $x = s$. At the first iteration, a straight line approximation was used. This approximation was iteratively improved, until either

1. a preset error tolerance for the Neumann condition was met and the iterative procedure terminated;

2. the change in the potential at each knot was below a preset tolerance. In this case, more spline segments were added and the iterative procedure continued.

The stability of the iterative scheme is strongly influenced by the choice of the quasi Newton constant, C. After some experimentation, a value of $C = 0.5$ was chosen for two spline segments, and a value of $C = 0.1$ was chosen for three or more spline segments, for the results presented in this paper.

Given a value for the potential function, the series coefficients A_n in (16) can be evaluated, using an orthogonality relationship. Noting that the potential at iteration i is given by $\bar{\phi}^{(i)}(x)$, then

$$A_n = \frac{2}{s\cosh(n\pi/s)} \int_0^s \left(\bar{\phi}^{(i)}(x) - h_1 - \frac{x(h_2 - h_1)}{s} \right) \sin \frac{n\pi x}{s}\, dx \qquad (41)$$

These integrals can be evaluated analytically or numerically. In the results given in this paper, the integrals were calculated numerically using the Matlab routine `quad8`.

The series solution is truncated, after sufficient terms have been included. The root-mean-squared error (rms) ε_g of the approximation of $g(x)$ by $\hat{g}(x)$ is defined to be

$$\varepsilon_g = \left(\frac{1}{s} \int_0^s \left(g(x) - \hat{g}(x) \right)^2 \, dx \right)^{\frac{1}{2}} \qquad (42)$$

For the example given in this paper, 10–20 terms were sufficient to produce rms errors in the range 10^{-2}–10^{-3} for the potential approximation.

Solutions were obtained for a number of parameter values and recharge distributions. Typically, 5–10 iterations were required for two spline segments, and a further 10–20 iterations were required when three to five spline segments were considered necessary to achieve sufficient accuracy. The rms errors in the stream function approximation were of the same order (10^{-2}–10^{-3}), except where there appeared to be a discontinuity in the stream function. For these cases, the errors were an order of magnitude larger.

Figure 1 and Figure 2 show streamline plots for typical solutions, with $s = 1$, $a = 0.5$ The recharge distribution used for Figure 1 was $r(x) = 0.05(x - 0.5)^2 - 1.24, \quad 0.5 \leq x \leq 1$, while the recharge distribution used for Figure 2 was $r(x) = -1.66\,x^2 + 3.32\,x - 0.25, \quad 0.5 \leq x \leq 1$. Due to space limitations, further flow plots have not been included.

7 Discussion

The similarities between the mathematical description of the free boundary and mixed boundary value problems leads to an iterative solution method for the mixed boundary value problem. In addition, the similarities continue during the iterative process. I found that all of the techniques that are useful for free boundary problems were also applicable to the mixed boundary prob-

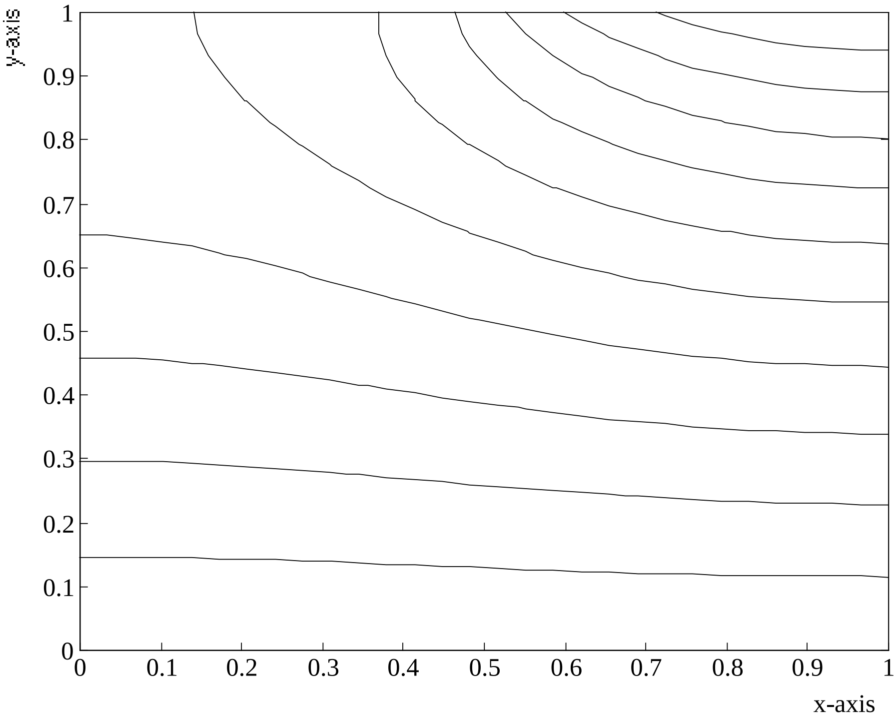

Figure 2: Flow solution using $r(x) = -1.66x^2 + 3.32x - 0.25, \quad 0.5 \le x \le 1$

lems. The is also a strong relationship between the numerical behaviour of both types of problem. For example, convergence can be poor for free boundary problems when the point updates (29) are used in the Quasi-Newton scheme. An exactly analogous behaviour was found for the iterative scheme for the mixed boundary value problem.

Another algorithmic similarity is in the values of the Quasi-Newton constant, C. In both types of problem, as the number of spline segments increases, C must be decreased. I found that the range of values that worked best for free boundary problems were also the values that worked best for the mixed boundary problem.

The behaviour of both schemes is very similar, when there are discontinuities present. Although it is beyond the scope of this paper, the methods that have been developed to work when discontinuities are present in the free boundary problem should also work for the mixed boundary problem. However, note that we don't know in advance if a discontinuity will be present, for the mixed boundary problem. This and other point on the mixed boundary value problem will be the focus of future research.

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