A series method for the eigenvalues of the advection diffusion equation

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Abstract

In steady hill slope seepage problems, the advection diffusion equation can be conformally transformed to a semi-regular solution domain using (ϕ, ψ) coordinates. Uniform flow in the (ϕ, ψ) domain reduces the advection diffusion equation to a simpler version with constant coefficients. The solutions depend on finding the eigenvalues (or *natural frequencies*) of an (elliptic) Helmholtz equation. In the absence of natural frequencies, this equation can be solved for nonzero boundary conditions using analytic series methods. In this paper, we present a pseudo-spectral approach to solve for the series coefficients. At the natural frequencies, the determinant of the coefficient matrix becomes zero, thus marking the natural frequencies. We present some preliminary results and identify natural frequencies for a set of test problems.

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1 Introduction

The management and conservation of subsurface water resources is extremely important in the current environmentally conscious society. Quantitative knowledge of the advection and diffusion processes of solutes through saturated aquifers is crucial in the development of effective management policies. This is particularly true in a relatively dry country like Australia, where groundwater is an essential natural resource. For example, solute transport can occur when increases in the water table elevation are caused by the removal of large surface vegetation, followed by the introduction of irrigated agriculture. More generally, contaminants can be carried from any surface source, through the vadose zone and across the water table, to then be transported though the groundwater system.

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The advective-diffusive process is governed by the flow equation and the transport equation. It can be extremely difficult to obtain accurate solutions to the transport equation, even when the flow field is known precisely. This problem is heightened by the large length to depth ratios common in most practical problems. Analytical solutions are available for regular infinite and semi-infinite flow domains, where the seepage velocity is constant [1, 2]. However, in practice aquifers are of irregular, finite shape and the seepage velocities are usually not uniform.

Analytic series solutions for the flow equations are obtained for steady seepage through irregular flow domains [3, 4, 5, 6]. As a consequence, the flow field are accurately and efficiently determined throughout the entire flow domain, and attention focused on solving the transport equation. For problems in two dimensions, both the potential solution ϕ and the conjugate stream function ψ are immediately available. Together they form an orthogonal curvilinear coordinate system in which the flow field is uniform. Thus the advection diffusion equation is conformally transformed to a uniform flow domain, using (ϕ, ψ) coordinates [4].

To solve the advection diffusion equation we apply separation of variables to the transformed problem, reducing it to an eigenvalue problem. After a simple transformation, we obtain the Helmholtz equation $\nabla^2 \varphi + \lambda \varphi = 0$. When λ is not an eigenvalue, this equation is solved using analytic series methods with non-zero boundary conditions. At the eigenvalues, the coefficient matrix (for the series coefficients) is singular, and the equation cannot be solved. In this paper, we develop a pseudo-spectral method to determine the matrix equation for the series coefficients. We present the eigenvalue spectra for five test problems, and discuss these results.

This paper is organised as follows. In Section 2, a formal mathematical description of the problem is given, together with details of the transformation process. The series solution method is described in Section 3, followed by the test problem results in Section 4.2. Finally, the method and results are discussed in Section 5.

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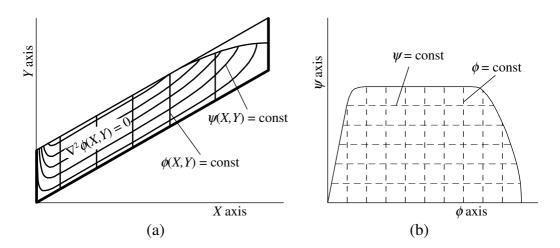


FIGURE 1: Schematic of the flow domain (a) and transformed domain (b)

2 Mathematical Problem Description

The flow problem in the original coordinates reduces to solving Laplace's equation $\nabla^2 \phi = 0$ for the hydraulic head $\phi(X,Y)$, subject to suitable boundary conditions. Analytic series solutions are readily obtained for saturated and steady seepage for almost arbitrary flow domain geometries and seepage rates [3, 5, 6]. Due to the analytic nature of the solution, the conjugate stream function $\psi(X,Y)$ is also immediately available. Both ϕ and ψ are available continuously throughout the flow domain, and together form an orthogonal coordinate system. A schematic of the original flow domain in the (X,Y) coordinate system and the transformed domain in the (ϕ,ψ) system is given in Figure 1. Typically, lengths in the X direction may be two orders of magnitude larger than those in the Y direction. In Figure 1(a), the X axis has been scaled and so the contours ϕ = constant and ψ = constant do not appear to be orthogonal as would normally be the case.

2.1 The advection diffusion equation

In the (X,Y) coordinate system, the advection diffusion equation for the concentration C(X,Y,t) is [2]

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial X} \left(D_{XX} \frac{\partial C}{\partial X} \right) + \frac{\partial}{\partial X} \left(D_{XY} \frac{\partial C}{\partial Y} \right) + \frac{\partial}{\partial Y} \left(D_{YX} \frac{\partial C}{\partial X} \right) + \frac{\partial}{\partial Y} \left(D_{YY} \frac{\partial C}{\partial Y} \right) - u \frac{\partial C}{\partial X} - v \frac{\partial C}{\partial Y}, \tag{1}$$

where the velocity field

$$\mathbf{u} = (u, v) = -\nabla\phi, \qquad (2)$$

(and with $\bar{u} = |\mathbf{u}| = \sqrt{u^2 + v^2}$). For diffusivities of the form $D_{\alpha\beta} = d_{\alpha\beta}^0 + d_{\alpha\beta}^1 \bar{u}$, where the $d_{\alpha\beta}^i$ are constant, equation (1) transforms to

$$\frac{1}{\bar{u}^2} \frac{\partial C}{\partial t} = \frac{\partial}{\partial \phi} \left(D_\phi \frac{\partial C}{\partial \phi} \right) + \frac{\partial}{\partial \psi} \left(D_\psi \frac{\partial C}{\partial \psi} \right) + \frac{\partial C}{\partial \phi}$$
 (3)

in the (ϕ, ψ) system [1, 4]. The coefficient of the advection term is positive, not negative—this is due to the negative potential in equation (2). As a first approximation, \bar{u} is taken to be a constant throughout the flow domain. This is a good approximation except near the water table and the seepage face. Equation (3) becomes

$$\frac{1}{\bar{u}^2} \frac{\partial C}{\partial t} = D_\phi \frac{\partial^2 C}{\partial \phi^2} + D_\psi \frac{\partial^2 C}{\partial \psi^2} + \frac{\partial C}{\partial \phi} \,. \tag{4}$$

2.2 Modal solutions

We represent the solution to equation (4) as a sum of modal solutions $\sigma_n(\phi, \psi)$ that are independent of t:

$$C(\phi, \psi, t) = \sum_{n=0}^{\infty} A_n \sigma_n(\phi, \psi) e^{-\bar{u}^2 \gamma_n^2 t}.$$
 (5)

Substituting into equation (4), we find that σ_n satisfies

$$D_{\phi} \frac{\partial^2 \sigma_n}{\partial \phi^2} + D_{\psi} \frac{\partial^2 \sigma_n}{\partial \psi^2} + \frac{\partial \sigma_n}{\partial \phi} + \gamma_n^2 \sigma_n = 0.$$
 (6)

This equation is transformed to the Helmholtz equation by the independent variable transformation

$$\phi = \sqrt{D_{\phi}}x, \quad \psi = \sqrt{D_{\psi}}y, \tag{7}$$

followed by the dependent variable transformation

$$\sigma_n(x,y) = e^{-x/2\sqrt{D_\phi}}\varphi_n(x,y).$$
 (8)

After these transformations, $\varphi_n(x, y)$ satisfies

$$\nabla^2 \varphi_n(x, y) + \lambda_n \varphi_n(x, y) = 0, \qquad (9)$$

where

$$\lambda_n = \gamma_n^2 - \frac{1}{2\sqrt{D_\phi}} \,. \tag{10}$$

In principle, the general solution to the original problem can be obtained once the eigenvalues and eigenfunctions of equation (9) have been obtained for the transformed flow geometry. In fact, it may turn out that the functions $\sigma_n(x,y)$ are not well-conditioned. This in turn means that the coefficients A_n in the expansion for C may be large and that equation (5) for the time development of C will rely on cancellations of large numbers. This issue has been discussed by Reddy and Trefethen [7].

3 Series Solution

For any fixed value of λ , solutions to the Helmholtz equation (9) are obtained using series methods. (Such solutions will generally not satisfy the boundary

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conditions.) Applying separation of variables, we assume a solution of the form

$$\varphi(x,y) = X(x)Y(y). \tag{11}$$

After substitution into the differential equation, we obtain two ordinary differential equations for X(x) and Y(y):

$$X_k'' + \mu_k X_k = 0, \quad Y_k'' - (\mu_k - \lambda) Y_k = 0,$$
 (12)

where μ_k is a constant of separation. If homogeneous boundary conditions are imposed on the side boundaries at $x = x_0$ and $x = x_1$, that is,

$$a_0 X_k(x_0) + b_0 X'_k(x_0) = 0$$
, $a_1 X_k(x_1) + b_1 X'_k(x_1) = 0$, (13)

then the eigenfunctions $X_k(x)$ and the constant of separation μ_k are determined. Furthermore, if we assume that $\varphi(x,y)$ is zero on the bottom boundary, y=0, then the solution for $\varphi(x,y)$ is written as

$$\varphi(x,y) = \sum_{k=1}^{\infty} A_k v_k(x,y), \qquad (14)$$

where $v_k(x,y) = X_k(x)Y_k(y)$. The expansion coefficients A_k are obtained from the top boundary condition. That is, along $y = f^t(x)$,

$$h^{t}(x) = \sum_{k=1}^{\infty} A_{k} v_{k}(x, f^{t}(x)) = \sum_{k=1}^{\infty} A_{k} v_{k}^{t}(x),$$
 (15)

for some function $h^t(x)$ (not necessarily zero).

3.1 Evaluation of the series coefficients

In this paper, we take a pseudo-spectral approach to evaluate the series coefficients A_n . First, we truncate the series after N terms, and collocate

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along the top boundary at N collocation points x_i , i = 1, ..., N:

$$h^{t}(x_{i}) = \sum_{k=1}^{N} A_{k} v_{k}^{t}(x_{i}), \text{ for } k = 1, \dots, N.$$
 (16)

In matrix form

$$V^t \mathbf{a} = \mathbf{h}^t \,, \tag{17}$$

where, for i, k = 1, 2, ..., N,

$$V_{ik}^t = v_k^t(x_i), \quad \mathbf{h}_i^t = h^t(x_i), \quad \mathbf{a}_i = A_i.$$
(18)

The matrix equation (17) can always be solved, unless the collocation matrix V^t is singular. In the case of homogeneous boundary conditions, non-trivial solutions will exist only if V^t is singular. We assume that this can only occur when λ is an eigenvalue or natural frequency of the Helmholtz equation (9), and (14) is an eigenfunction.

4 Results

We examine the effectiveness of this method on a test problem related to (but not the same as) the transformed flow domain given in Figure 1. We choose a sequence of five test geometries, and compare the evolution of the eigenvalue spectrum as we progressively move from a known problem to the final geometry.

4.1 Test problems

The geometry of the test problems is related to the unit square whose eigenvalues are readily determined. The bottom boundary and side boundaries are the same for each of the five test problems, namely

$$y = 0$$
, $0 \le x \le 1$; $x = 0$, $0 \le y \le w$; $x = 1$, $0 \le y \le w$. (19)

The five top boundaries are

$$y = f^{t}(x, w) = w + 4(1 - w)x(1 - x), \quad w = 0:0.25:1.$$
 (20)

Note that for w = 1, the test problem corresponds to the unit square, and for w = 0, the upper boundary is a quadratic of height one, symmetric about x = 0.5. In this last case, the vertical side boundaries only apply at the corners (0,0) and (1,0)—even though they appear to be irrelevant, we use them to fully define the eigenvalue/eigenfunction problem in equations (12) and (13). The five flow geometries are shown in Figure 2.

Given the boundaries, the problem will be fully defined once the boundary values of $\varphi(x,y)$ are given. In this paper, we choose Dirichlet boundary conditions. That is,

$$\varphi(0,y) = \varphi(1,y) = 0, \qquad 0 \le y \le w; \tag{21}$$

$$\varphi(x,0) = \varphi(x, f^t(w,x)) = 0, \quad 0 \le x \le 1.$$
 (22)

4.2 Test Spectra

For the boundary geometry and conditions given in Section 4.1, $\mu_k = k^2 \pi^2$ and the expansion functions $v_k(x, y)$ in equation (14) become

$$v_k(x,y) = Y_k(y)\sin k\pi x, \qquad (23)$$

where

$$Y_k(y) = \begin{cases} \sin \gamma_k y, & k \le n_0, \\ \sinh \gamma_k y/\cosh \gamma_k, & k > n_0, \end{cases}$$
 (24)

with

$$\gamma_k^2 = |\lambda - k^2 \pi^2|$$
 and $n_0 = \left| \frac{\sqrt{\lambda}}{\pi} \right|$ (25)

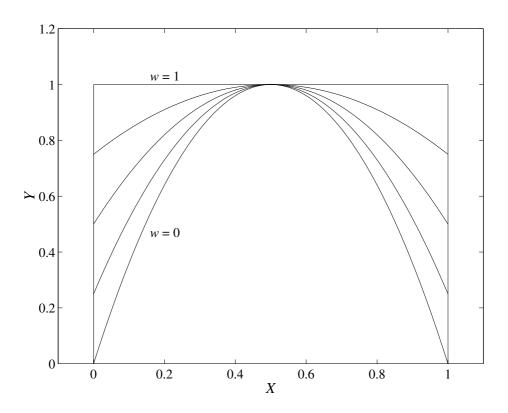


FIGURE 2: Flow geometries for the five test problems

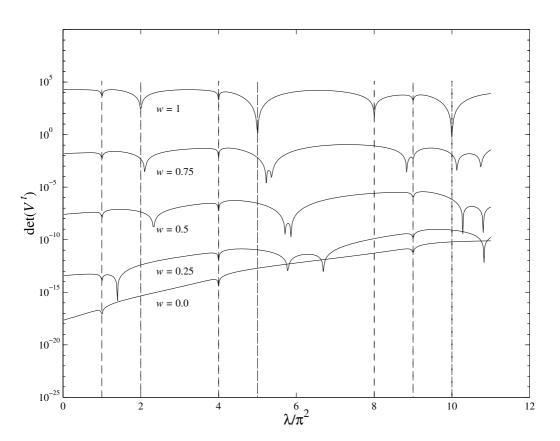


FIGURE 3: The spectra for the five test geometries. The vertical lines give the known eigenvalues for w=1 (the "box" example).

Note that $\cosh \gamma_k$, a scaling term for $Y_k(y)$, $k > n_0$, is used to improve the conditioning of the collocation matrix. Since equation (23) is an expansion in sine functions, equally spaced collocation points appear to be the best choice for this set of test problems. We use eleven terms (N = 11) in the truncated series approximation (equation (14)) for $\varphi(x, y)$.

We now calculate the determinant of the collocation matrix V^t for a contiguous set of values of λ —at the natural frequencies of each problem, the determinant will approach zero. The eigenvalues λ_{mn} of the Helmholtz equation (9) for the unit square with Dirichlet boundary conditions are

$$\frac{\lambda_{mn}}{\pi^2} = m^2 + n^2, \quad m, n = 1, 2, \dots$$
 (26)

The first eight eigenvalues are 2, 5, 8, 10, 13, 17, 18, 20. To test the approach developed in this paper, we use 503 equally spaced values of λ , $0 < \lambda/\pi^2 \le 20$. We choose 503 points (rather than 500) so that λ does not fall exactly on an eigenvalue of the first test problem. The magnitude of the determinant for each of the five test problems is given in Figure 3.

5 Discussion

We have shown how an analytic series method is used to obtain approximations to the eigenvalues of the Helmholtz equation with homogeneous boundary conditions on non-rectangular boundaries. The next stage in the problem is to obtain the solutions for φ from the solution of $V^t \mathbf{a} = \mathbf{0}$ for each of the eigenvalues.

At this stage it is interesting to note some of the features of the results in Figure 3. For the problem defined on a rectangular domain (w=0), the frequencies are given by equation (26). There are three types of frequencies. The frequencies with m or n equal to zero have been labelled irregular frequencies. They correspond to $\varphi \equiv 0$. These 'solutions' do not appear if

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the 'method of particular solutions' as described by Betcke and Trefethen [8] is used. Those frequencies with m = n are single frequencies. Those with $m \neq n$ are double frequencies. These different types of frequency change in different ways with the changes in geometry.

See that the irregular frequencies remain at the same values $(\lambda/\pi^2 = 1, 4, 9, ...)$ as for the rectangular domain. The single frequencies $(\lambda/\pi^2 = 2, 8, ...)$ for the rectangular domain) increase as the value of w is reduced. The double frequencies $(\lambda/\pi^2 = 5, 10, ...)$ also increase, but at the same time they bifurcate into two separate frequencies as w decreases. Some of these features are absent for w = 0. We believe that this is a result of low resolution in the values of λ , rather than any fundamental difference in the solution for that value. This and other issues raised in this paper are topics of current research.

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