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Exact Matching of Boundary Conditions and Incorporation of Semiquantitative Solution Characteristics in Initial Approximations to Boundary Value Problems

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Methods are described and illustrated which permit the analyst to construct initial approximations which match virtually any type of boundary condition exactly while also permitting the specification of certain auxiliary constraints such as convexity or the satisfaction of a maximum principle. These methods are based upon transfinite or blending-function interpolation. Such initial approximations are then used to substantially improve the computational efficiency of iterative solution techniques.

1. INTRODUCTION

The engineering analyst confronted with a boundary value problem most often has substantially more information about the behavior of the solution than the quantitative information required to guarantee that the problem is mathematically well posed. This information may be of a heuristic or semiquantitative nature and known to the analyst only by virtue of his understanding of the underlying physical principles or past experience with similar problems. The purpose of this note is to describe and illustrate simple techniques which permit the analyst to quantitatively exploit such auxiliary information and thereby substantially improve the computational efficiency of an iterative numerical solution technique.

More specifically, the proposed methods are based upon the notion of *blending-function interpolation* and are designed to guarantee the *exact* satisfaction of boundary conditions while also permitting the specification of certain auxiliary constraints such as convexity or the satisfaction of a maximum principle.

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2. Reduction of Nonhomogeneous to Homogeneous Boundary Conditions

Standard finite difference or finite element methods for the numerical solution of boundary value problems are only able to satisfy general nonhomogeneous boundary data at a finite number of nodal or mesh points. In this section we describe a constructive technique whereby a given boundary value problem with nonhomogeneous boundary conditions can be transformed into an equivalent boundary value problem having homogeneous boundary conditions. The function which we construct to accomplish this reduction of boundary values is a blended or transfinite interpolant [3, 6] which exactly matches the given boundary data.

The Marshall–Mitchell approach [9] also accomplishes the goal of exactly matching Dirichlet boundary data. More recent papers exploit blending-function interpolation schemes to exactly accommodate Neumann data for second-order elliptic problems [8], and the essential boundary conditions (i.e., function value and normal derivatives) for fourth-order elliptic problems [10]. However, the methods developed in [8–10] differ conceptually from the approach proposed here in the respect that they are based upon a strategy which laces the boundary of the problem domain with special elements designed to satisfy the boundary conditions along the outer perimeter of each of the elements. In contrast to this *local* element-by-element strategy, the class of methods described below are *global* in the sense that a smooth boundary condition interpolant is constructed over the entire problem domain *before* the boundary value problem is discretized for numerical solution.

We first restrict our attention to the unit square $\mathscr{S}$ and later indicate how more general domains might be handled. Let $\mathscr{L}$ be a second-order differential operator and consider the boundary value problem

$$\mathscr{L}[u] = f \qquad (x, y) \in \mathscr{S} = [0, 1] \times [0, 1] \tag{1}$$

subject to Dirichlet boundary conditions

$$u = g \qquad (x, y) \in \partial\mathscr{S}. \tag{2}$$

We shall assume that this is a well-posed boundary value problem.

Since discrete models (finite difference or finite element) can exactly match *homogeneous* boundary conditions, but not general nonhomogeneous conditions, our strategy is as follows.

(i) Construct a function U_0 which satisfies the *nonhomogeneous* boundary conditions (2) and which is smooth enough so that $\mathscr{L}[U_0]$ is defined.

(ii) Apply $\mathscr{L}$ to the residual function $u - U_0$ to obtain

$$\mathscr{L}[u - U_0] = \bar{f} \tag{3}$$

where $\bar{f} \equiv f - \mathscr{L}[U_0]$.

(iii) Solve the boundary value problem

$$\mathscr{L}[u_1] = \bar{f} \qquad (x, y) \in \mathscr{S} \tag{4}$$

subject to the homogeneous boundary conditions

$$u_1 = 0 \qquad (x, y) \in \partial\mathscr{S} \tag{5}$$

using a finite element or finite difference program to obtain an approximation U_1 to u_1.

(iv) Construct $U = U_0 + U_1$ as the approximation to U, the solution to the original boundary value problem (1), (2).

We note that steps (i) and (ii) are performed in a *preprocessing* stage and step (iv) in a *postprocessing* stage. Thus, an existing finite element or finite difference computer program may be used without modification to compute the approximation U_1 in step (iii).

In brief, the idea is that one can easily construct a first approximation U_0 which matches the boundary conditions and, perhaps, auxiliary conditions which the analyst wishes to impose. In practice, we seek to incorporate into U_0 as much information as possible regarding the behavior of the true solution u. For instance, if $\mathscr{L}$ is the Laplacian, then it is well known that $\max | u | \leq \max_{\partial\mathscr{S}} | u |$ (Maximum Principle), so that we would attempt to somehow incorporate this condition into the first approximation U_0 (see Examples 2 and 3). Physical considerations or the analyst's experience may provide other qualitative or semiquantitative insights which may be quantified and incorporated into the function U_0.

The reader may note that our proposed strategy of first nullifying the boundary conditions and reducing the original problem to an equivalent problem with homogeneous boundary conditions is the standard approach used in the development of the variational theory of linear partial differential equations [12, p. 101; 11, p. 163]. However, in such theoretical developments, one is not concerned with the actual *constructibility* of U_0. It is precisely the question of constructibility that we address in this paper.

To begin, we recall that blended bivariate interpolation [1–6] readily yields a solution to the following problem. Given the boundary functions $u(0, y)$, $u(1, y)$, $u(x, 0)$, and $u(x, 1)$ construct a function U_B on the unit square such that U_B matches these boundary conditions. The simplest solution to this problem is the *bilinearly blended* interpolant

$$\begin{aligned} U_B(x, y) = {} & (1 - x)\, u(0, y) + xu(1, y) \\ & + (1 - y)\, u(x, 0) + yu(x, 1) \\ & - (1 - x)(1 - y)\, u(0, 0) - (1 - x)\, yu(0, 1) \\ & - x(1 - y)\, u(1, 0) - xyu(1, 1). \end{aligned} \tag{6}$$

It is easy to verify that U_B possesses derivatives to the same order as the boundary functions and satisfies the requisite boundary condition

$$U_B = g \qquad (x, y) \in \partial\mathscr{S}.^1$$

[1] We assume that $u(0, 0) = u(0, y)_{y=0} | = u(x, 0)_{x=0} |$, etc.

We hence choose $U_0(x, y) = U_B(x, y)$ as a first approximation to the solution of our boundary value problem.

The domain transformations discussed by Gordon and Hall [5] can be used in conjunction with (6) to accomplish the same construction over nonrectangular domains. If the domain R is that shown in Fig. 1, then the notions of *transfinite* mapping and interpolation [5, 6] provide a means of easily constructing a function U_0 with domain R which matches given boundary data on ∂R. (For details of this example, see [5, p. 475]). The methods described in these two earlier papers can be used either directly or with slight adaptation to treat most regions of practical interest.

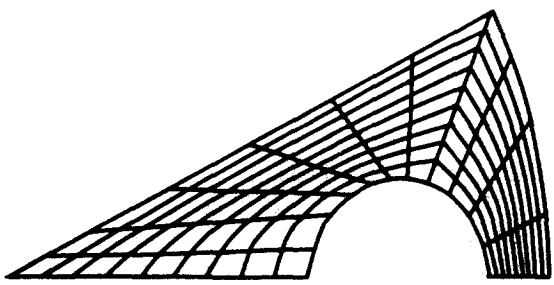


FIG. 1. Constant s and t coordinate lines relative to an induced natural coordinatization of this domain with curved boundaries (cf. [5, p. 475]). An initial approximation $U_0(s, t)$ can be constructed as the bilinearly blended interpolant of Dirichlet data.

It is also easy to handle nonhomogeneous Neumann or mixed type boundary conditions. For example, suppose $\mathscr{L}$ is the Laplace operator (∇^2) and the boundary conditions on $\partial\mathscr{S}$ are

$$\begin{aligned} u &= g_1, & x &= 0,\ 0 \leq y \leq 1, \\ u &= g_2, & y &= 1,\ 0 \leq x \leq 1, \\ u &= g_3, & y &= 0,\ 0 \leq x \leq 1, \\ u_x + \sigma u &= g_4, & x &= 1,\ 0 \leq y \leq 1,^2 \end{aligned} \tag{7}$$

The boundary conditions in (7) can be reduced to homogeneous conditions and accounted for in the computer model by modifying the source as in (4) where now U_0 is constructed as follows.

(i) Choose an approximation $\tilde{u}(1, y)$ to the unknown boundary function $u(1, y)$; for example, one may take the straight-line interpolant

$$\tilde{u}(1, y) = yu(1, 1) + (1 - y)\, u(1, 0). \tag{8}$$

[2] We assume that the boundary conditions are compatible in the sense that $g_1(0) = g_3(0) = u(0, 0)$, $g_1(1) = g_2(0) = u(0, 1)$, etc. However, with slight adaptation these same techniques can also be applied to problems with discontinuous or incompatible boundary conditions.

The associated approximation to the flux u_x along the boundary $x = 1$ is from (7),

$$\tilde{u}_x(1, y) = g_4(y) - \sigma\tilde{u}(1, y) \qquad 0 \leq y \leq 1. \tag{9}$$

(ii) Construct the blended surface (quadratically blended in x and linearly blended in y)

$$\begin{aligned} U_{QL}(x, y) = {} & yg_2(x) + (1 - y)g_3(x) \\ & + (x - 1)^2 g_1(y) + x(2 - x)\tilde{u}(1, y) - x(1 - x)\tilde{u}_x(1, y) \\ & - y(x - 1)^2 g_1(1) - yx(2 - x)g_2(1) - yx(1 - x)\tilde{u}_x(1, 1) \\ & - (1 - y)(x - 1)^2 g_1(0) - (1 - y)x(2 - x)g_3(1) \\ & - (1 - y)x(1 - x)\tilde{u}_x(1, 0). \end{aligned} \tag{10}$$

Then, it is easy to check that U_{QL} satisfies the nonhomogeneous boundary data (7). We choose $U_0(x, y) = U_{QL}(x, y)$ and $v = u - U_0$ so that we have

$$\mathscr{L}[v] = f - \mathscr{L}[U_0] \tag{11}$$

subject to homogeneous data

$$\begin{aligned} u &= 0 \qquad \text{for} \quad x = 0,\ 0 \leqslant y \leqslant 1 \text{ and } y = 0,\ 1,\ 0 \leqslant x \leqslant 1, \\ u_x + \sigma u &= 0 \qquad \text{for} \quad x = 1,\ 0 \leqslant y \leqslant 1. \end{aligned} \tag{12}$$

In practice, the analyst may have additional insight regarding the behavior of the solution u and may be able to use this information to better estimate the boundary function $u(1, y)$. Note that relations (9) and (10) provide a function which satisfies the boundary conditions (7) for *any* choice of $\tilde{u}(1, y)$.

Note too that, in contrast to the variational formulation of the original problem, the variational formulation of (11) subject to (12) involves no boundary integrals. Even for direct solution methods, this can be an advantage of the proposed method if the boundary value problem is to be solved via finite element methods since exact satisfaction of boundary conditions eliminates one of the major sources of numerical error in finite element models. However, in the present paper we shall not explore these potential advantages for direct methods.

As a specific illustration of the proposed technique for obtaining first approximations which exactly match boundary conditions *and* incorporate auxiliary information regarding the behavior of the solution, consider Laplace's equation over $\mathscr{S}$ with Dirichlet boundary conditions. By virtue of the Maximum Principle for harmonic functions we would expect that the value of the solution at the center of the square might be well approximated by the average of the boundary values, viz.,

$$\begin{aligned} \tilde{u}(\tfrac{1}{2}, \tfrac{1}{2}) = 0.25 \Big\{ & \int_0^1 u(0, y)\, dy + \int_0^1 u(1, y)\, dy \\ & + \int_0^1 u(x, 0)\, dx + \int_0^1 u(x, 1)\, dx \Big\}. \end{aligned} \tag{13}$$

To illustrate how one constructs a boundary interpolant which also satisfies condition (13), suppose that we first nullify the Dirichlet boundary conditions by subtracting from the (as yet unknown) initial approximation U_0 the bilinearly blended interpolant U_B of (6). Then, we have that

$$U_0(\tfrac{1}{2}, \tfrac{1}{2}) - U_B(\tfrac{1}{2}, \tfrac{1}{2}) = \tilde{u}(\tfrac{1}{2}, \tfrac{1}{2}) - U_B(\tfrac{1}{2}, \tfrac{1}{2}) \tag{14}$$

the right-hand side of which is computable from the given boundary conditions and Eqs. (6) and (13). Now, we seek a "correction" function $v(x, y)$ which vanishes on the perimeter of $[0, 1] \times [0, 1]$ and achieves the value $\tilde{u}(\frac{1}{2}, \frac{1}{2}) - U_B(\frac{1}{2}, \frac{1}{2})$ at the point $(x, y) = (\frac{1}{2}, \frac{1}{2})$. Such a function is easy to construct. For instance, the simplest function having the requisite properties is biquadratic

$$v(x, y) = 16x(1 - x)\, y(1 - y)[\tilde{u}(\tfrac{1}{2}, \tfrac{1}{2}) - U_B(\tfrac{1}{2}, \tfrac{1}{2})]. \tag{15}$$

It is easy to verify that the function

$$U_0(x, y) = U_B(x, y) + v(x, y) \tag{16}$$

satisfies

$$\begin{aligned} U_0(0, y) &= u(0, y), \qquad U_0(1, y) = u(1, y), \\ U_0(x, 0) &= u(x, 0), \qquad U_0(x, 1) = u(x, 1), \end{aligned} \tag{17}$$

and

$$U_0(\tfrac{1}{2}, \tfrac{1}{2}) = \tilde{u}(\tfrac{1}{2}, \tfrac{1}{2}).$$

In Example 2 below we will use this function to demonstrate the efficacy of the proposed approximation scheme in enhancing the efficiency of the iterative numerical solution of Laplace's equation.

Under certain conditions, the initial approximation U_0 will be the exact solution to the given boundary value problem (1), (2). To see how this comes about, recall that blended interpolation schemes are uniquely characterized by certain types of partial differential equations [1, 3] or by a variational principle [4]. For instance, bilinearly blended interpolation (6) is characterized as being the unique $C^{(2,2)}$ function which matches the Dirichlet boundary conditions on $\mathscr{S}$ and satisfies the fourth-order hyperbolic differential equation $\partial^4 U_B/\partial x^2 \partial y^2 = 0$, which in [1] was termed the Draftsman's equation. Similarly, the blended interpolant (10) can be characterized as the unique function in $C^{(3,2)}$ which interpolates the four boundary curves plus the normal derivative along $x = 1$ and satisfies the differential equation $\partial^5 w/\partial x^3 \partial y^2 = 0$.

As an example, consider the partial differential equation

$$-\nabla^2 u + 9u = 0 \qquad (x, y) \in \mathscr{S} \tag{18}$$

with Dirichlet boundary conditions

$$\begin{aligned} u(0, y) &= 1 + e^{-3y}, \qquad u(1, y) = e^3 + e^{-3y}, \\ u(x, 0) &= 1 + e^{3x}, \qquad u(x, 1) = e^{-3} + e^{3x}. \end{aligned} \tag{19}$$

Let us construct the function (6) which matches these boundary conditions

$$\begin{aligned} U_B(x, y) &= (1 - x)[1 + e^{-3y}] + x[e^3 + e^{-3y}] \\ &\quad + (1 - y)[1 + e^{3x}] + y[e^{-3} + e^{3x}] \\ &\quad - (1 - x)(1 - y)(2) - (1 - x)y(e^{-3} + 1) \\ &\quad - x(1 - y)(e^3 + 1) - xy(e^{-3} + e^3) \\ &= e^{3x} + e^{-3y}. \end{aligned} \tag{20}$$

In accord with the procedure outlined above, we now use this function U_B to nullify the boundary conditions of the original problem and to obtain, in general, an inhomogeneous differential Eq. (4) subject to homogeneous boundary conditions (5) on the residual function $u_1 = u - U_B$. But, in this instance we find that

$$\mathscr{L}[u_1 + U_B] = (-\nabla^2 + 9)[u_1 + e^{3x} + e^{-3y}], \tag{21}$$

so that we are left with the boundary value problem

$$-\nabla^2 u_1 + 9u_1 = 0 \tag{22}$$

with

$$u_1 \equiv 0 \qquad \text{on } \partial\mathscr{S}.$$

The unique solution to this problem is $u_1 \equiv 0$ which shows that the bilinearly blended function U_B is the *exact* solution to the original boundary value problem (18), (19). Another way of expressing this fact is to say that the function $e^{3x} + e^{-3y}$ is in the intersection of the null spaces of the operators $\partial^4/\partial x^2 \partial y^2$ and $-\nabla^2 + 9$.

3. Initialization of Iterative Schemes

The systems of equations that arise in finite difference or finite element models of boundary value problems in two and three dimensions are often solved via iterative solution techniques [2, 13]. In this section we illustrate with several numerical examples how blended interpolation to boundary data and/or other auxiliary information can be useful in initializing such iterative schemes. In all of these examples the computational efficiency of the iterative solution method is enhanced, i.e., the number of iterations required to obtain a specified accuracy is significantly less than the number of iterations required using the simpler and more conventional initialization procedure of setting all unknown nodal values equal to a constant. Of course, the "rate of convergence" of the iterative scheme is unchanged. It is simply that we begin with a better first approximation.

Although the examples presented here are all linear boundary value problems the same technique is equally applicable to the solution of nonlinear problems. Indeed, because of the well-known difficulties in obtaining numerical solutions for such problems, the need for good initialization procedures is greater.

EXAMPLE 1. Consider the differential equation

$$-\nabla^2 u + 9u - f = 0 \qquad (x, y) \in \mathscr{S} \equiv [0, 1] \times [0, 1] \tag{23}$$

where $f(x, y) = 6xe^{-3y} - e^{-3x} \sin y$, subject to Dirichlet data on $\partial\mathscr{S}$. The true solution to this boundary value problem is $u(x, y) = e^{-x} \sin y + x^3 e^{-3y}$. The standard five-point finite difference approximation [2, p. 192] was used to find a discrete solution to this boundary value problem with a mesh gauge of $h = 1/21$. The linear system consisting of 400 equations was solved using the *Gauss–Seidel* iterative scheme [13, p. 57]. The L_∞-norm of the residual, $\| \underline{x}^{(k)} - \underline{x}^{(k-1)} \|_\infty$, was monitored as an indication of convergence of the sequence of iterates $\underline{x}^{(k)}$ to the solution x of the finite difference model. If $\underline{u}$ is the vector of values of the true solution u at the points of the finite difference grid, from the computations we observe that $\| \underline{x} - \underline{u} \|_\infty \approx 0.14 \times 10^{-4}$.

Two different initial guesses were used; first, the values of the grid function at interior points were set to one, i.e., $\underline{x}^{(0)} = \underline{1} = (1,\ldots, 1)^T$. Second, they were set to the values of the *bilinearly blended interpolant* (6) of the boundary data. We define U_B to be the vector of evaluations of U_B at the appropriate grid points. The convergence results are summarized in Fig. 2. The bilinearly blended initial guess resulted in the norm of the residual being less than 10^{-4} in 103 iterations compared to 187 iterations for the initial guess $\underline{1}$, i.e., *a* 45% *savings in the number of iterations.*

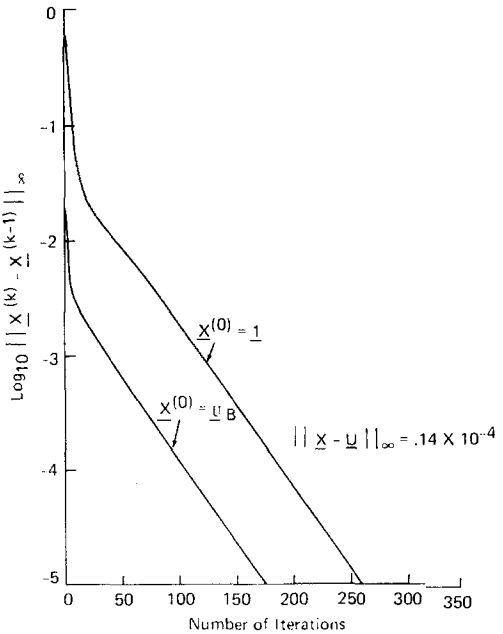


FIG. 2. $\| \underline{x}^{(k)} - \underline{x}^{(k-1)} \|_\infty$ for Example 1.

EXAMPLE 2. The standard five-point finite difference approximation was used again to solve Laplace's equation

$$\nabla^2 u = 0 \qquad (x, y) \in \mathscr{S} = [0, 1] \times [0, 1] \tag{24}$$

subject to Dirichlet data

$$\begin{aligned} u(x, 0) = u(x, 1) &= 4x(1 - x) \qquad 0 \leqslant x \leqslant 1, \\ u(0, y) = u(1, y) &= 4y(1 - y) \qquad 0 \leqslant y \leqslant 1. \end{aligned} \tag{25}$$

Two uniform grids were used, of gauge $h = 1/31$ and $h = 1/62$, respectively. The resulting systems of 900 and 3721 (resp.) equations were solved using the *successive overrelaxation* iterative scheme [13, p. 58] and the optimum relaxation factor $\omega = 2/(1 + \sin \pi h)$, [13, p. 203]. Each system was solved using the two initial guesses (i) $\underline{x}^{(0)} = \frac{2}{3}\underline{1}$ ($\frac{2}{3}$ being the value determined by (13)) and (ii) $\underline{x}^{(0)}$ determined as the value of the bilinearly blended interpolant (6) of the boundary data. The bilinearly blended surface is a poor first approximation to u since it assumes the value 2 at $(\frac{1}{2}, \frac{1}{2})$ and the maximum principle guarantees $\max_{\text{int}\mathscr{S}} |u(x, y)| < 1$. Thus, the bilinearly blended approximant $\underline{x}^{(0)} = \underline{U}_B$ yields little improvement over the initial approximation $\underline{x}^{(0)} = \frac{2}{3}\underline{1}$, cf. Figs. 3a, b.

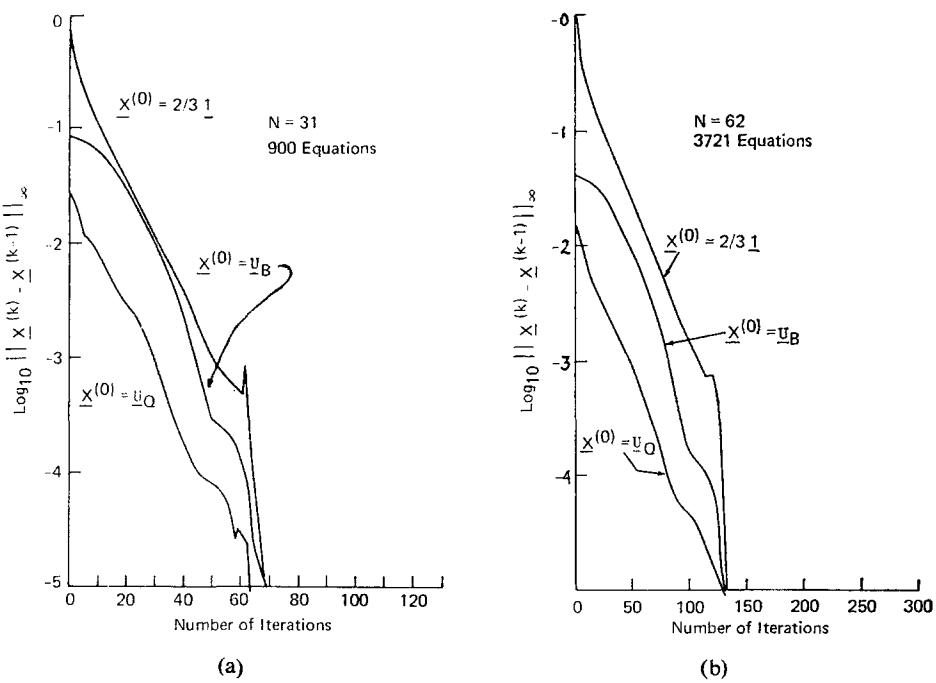
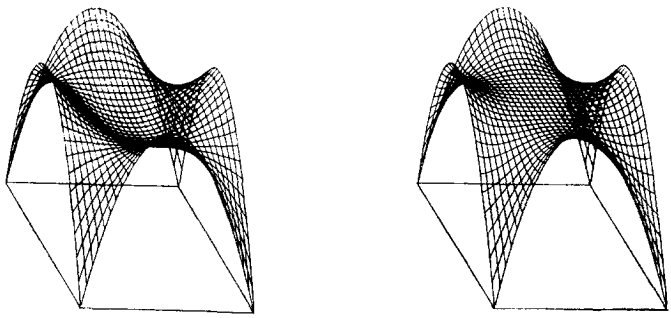


FIG. 3. a. Norm of residuals for Example 2. $N = 31$. b. Norm of the residuals for Example 2. $N = 62$.

The qualitative information implied by the maximum principle can be accounted for by the use of a third initial guess $\underline{x}^{(0)} = \underline{U}_Q$ where $\underline{U}_Q$ is the vector containing the evaluation of U_0 in (16) at the appropriate mesh points. Figures 4a, b illustrate how closely this initial approximation mimics the behavior of the actual solution.



(a) (b)

FIG. 4. a. Initial approximation $\underline{U}_Q$. b. Finite difference Approximation.

FIGURE 4. EXAMPLE 2. Initial approximation $\underline{U}_Q$ based on (13) and (16) which accounts for the maximum principle in comparison to the finite difference solution for $h = 1/31$. Note that from (13) we find $\tilde{u}(\frac{1}{2}, \frac{1}{2}) = \frac{2}{3}$. The incorporation into the initial guess of this "semiqualitative" information (i.e., the maximum principle) results in about a 25% reduction in the number of iterations required for convergence to 10^{-4}. This is true for both values of $N = 31$ and 62.

EXAMPLE 3. Next, we considered the differential equation $-\nabla^2 u + 9u = 0$ subject to the same boundary conditions as Example 2. The maximum principle also holds for the differential operator $-\nabla^2 u + 9u$. A mesh gauge of $h = 1/21$ was used and the Gauss–Seidel iterative method was used to solve the linear system. The results are summarized by Fig. 5. Note that, based on the finite difference approximation, the true solution u at $(\frac{1}{2}, \frac{1}{2})$ is approximately 0.46 in comparison to 0.82 for Laplace's equation of Example 2. The initial guess of $\frac{2}{3}\underline{1}$ is high at about as many mesh points as it is low in Example 3. In Example 2, in contrast, this estimate is too small for all but about 10% of the points clustered in the four corners. This explains why $\frac{2}{3}\underline{1}$ is a poor first approximation in Example 2, but a comparatively good estimate in Example 3.

On the basis of the results shown in Fig. 5, it is clear that our attempt to improve the fidelity of the initial iterate by the incorporation of auxiliary information (the maximum principle) was not successful in this example. To understand why this is true, note that the solution to $-\nabla^2 u + \alpha u = 0$ tends to $u = 0$ in the interior of the region as the parameter $\alpha \to \infty$. Hence, the solution u to $-\nabla^2 u + 9u = 0$ is relatively "flat" within the region $[0, 1] \times [0, 1]$, whereas the initial approximation given by

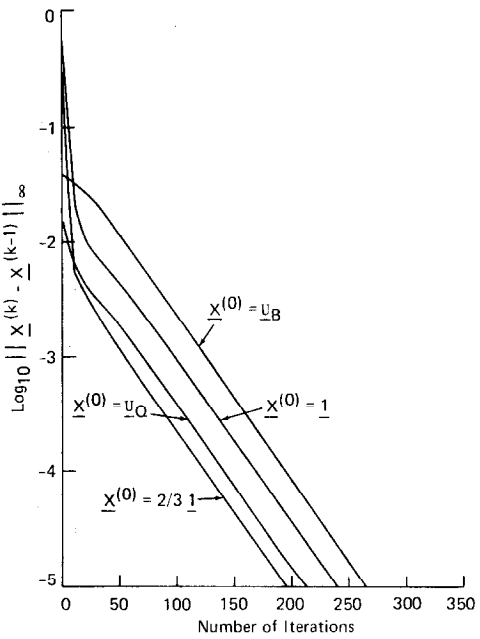


FIG. 5. $\| \underline{x}^{(k)} - \underline{x}^{(k-1)} \|_\infty$ for Example 3.

U_0 of (16) behaves much like the actual solution to Laplace's equation as shown in Fig. 4b. From this heuristic argument, we are able to deduce that in order to improve the initial iterate, we should employ not only our knowledge that u satisfies a maximum principle, but should also modify the function $v(x, y)$ in (15) so as to reflect the relative flatness of the solution to $-\nabla^2 u + 9u = 0$.

Two other examples are contained in a General Motors Technical Report GMR-2480 which was an earlier version of this paper. The first example concerns a non-model boundary value problem arising in the design of fluorescent lamps, cf. [7]. The finite difference equations are solved using the block Gauss–Seidel scheme which is initialized as suggested in this paper. The second example illustrates how the proposed procedure can be implemented when the domain is not a rectangle.

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