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ON FINITE ELEMENT DOMAIN IMBEDDING METHODS*

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Abstract. Finite element domain imbedding methods for the Helmholtz equation with Neumann and Dirichlet boundary conditions on nonrectangular domains in two space dimensions are considered. A survey and comparison of known methods are given, and a number of improvements suggested. Results of numerical experiments are also presented.

Key words. fast elliptic solvers, capacitance matrix methods

AMS(MOS) subject classifications. 65F10, 65N30, 65N50

1. Introduction. Domain imbedding methods are solvers of elliptic equations constructed in the following way. To solve an elliptic boundary value problem on a general bounded domain Ω in two or three space dimensions, an auxiliary boundary value problem is chosen on a larger, but simpler domain. A fast solver for the auxiliary problem is then used to construct a preconditioner for the original problem.

Methods of this kind are often called capacitance matrix methods in the West and fictitious domain methods in the Soviet Union. They have been studied extensively; see, for example, [1], [2], [6], [9], [10], [13]–[19]. A remarkably efficient multigrid-based domain imbedding method, quite different from the ones considered here, has also been proposed by Dendy in [8].

In this paper, we shall study imbedding methods for Neumann and Dirichlet problems for the Helmholtz equation on bounded domains Ω in the plane, using finite element discretizations. The region Ω is imbedded in a sufficiently large rectangle in such a way that $\overline{\Omega}$ does not intersect the boundary of the rectangle. For simplicity, we shall always assume that this rectangle is the unit square $(0,1)^2$.

The methods considered require triangulations of a special kind. In particular the vertices of the triangles should lie on a logically rectangular mesh. We outline such a triangulation algorithm in §3. Details can be found in [3] and [4].

An efficient iterative finite element imbedding method was introduced for the Neumann problem by Proskurowski and Widlund [17]. In each iteration, an auxiliary boundary value problem is solved on $(0,1)^2$. In §4 of this paper, we study the best choice of boundary values on $\partial(0,1)^2$ and the effect of using an inexact solver for the problem on the rectangle.

In §5, we consider an analogous method for the Dirichlet problem. In contrast with the method of §4, this method is nonoptimal, i.e., the number of iterations needed for a prescribed accuracy is not bounded uniformly in the mesh width. However, the method is simple, and we present some numerical results illustrating its performance.

In §6, we consider a method for Dirichlet problems on Ω which makes use of an auxiliary problem on $(0,1)^2 - \overline{\Omega}$ with Neumann conditions on $\partial\Omega$ and Dirichlet

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boundary conditions on $\partial(0,1)^2$. This method was proposed and studied by Dryja [9] and Widlund [21]. We show that it fails, for the Poisson equation, if the domain Ω is multiply connected, a fact apparently previously overlooked. We also propose a simple way of overcoming this difficulty.

This paper is based on the far more extensive technical report [4]. That report, and the codes used for our numerical experiments, are available from the authors. Our programs include an implementation of quadratic isoparametric elements.

2. Notation. Let Ω be a bounded domain in R^2 with a Lipschitz continuous boundary $\partial\Omega$. We will consider the Neumann problem

$$-\Delta u + cu = f \quad \text{on } \Omega \tag{1}$$

$$\frac{\partial u}{\partial n} = g \quad \text{on } \partial\Omega, \tag{2}$$

and the Dirichlet problem

$$-\Delta u + cu = f \quad \text{on } \Omega \tag{3}$$

$$u = g \quad \text{on } \partial\Omega. \tag{4}$$

$\partial/\partial n$ denotes the exterior normal derivative, and c a real constant. We assume that $c \geq 0$.

We use finite element discretizations based on triangles $\tau_1, \cdots, \tau_k$ and $\tau_{k+1}, \cdots, \tau_{2N^2}$ such that $(\tau_\nu)_{1\leq\nu\leq 2N^2}$ is a triangulation of $(0,1)^2$ and

$$\Omega^h := \bigcup_{1\leq\nu\leq k} \tau_\nu \tag{5}$$

approximates Ω. In this paper we only use piecewise linear Lagrangian finite elements. Results for piecewise quadratic isoparametric elements can be found in [4].

The degrees of freedom are the values of the finite element functions at the vertices of the triangles. We will make use of auxiliary boundary value problems on the entire square $(0,1)^2$, with boundary conditions on $\partial(0,1)^2$ specified later. The finite element discretization of these problems results in a system of linear equations

$$K(c)\underline{x} = \underline{r}, \tag{6}$$

with

$$K(c) = K + cM, \tag{7}$$

where K is the stiffness matrix and M is the mass matrix. The entries in K and M are of the form

$$\int_{[0,1]^2} \underline{\nabla}\phi^T \cdot \underline{\nabla}\psi d\underline{x} \tag{8}$$

and

$$\int_{[0,1]^2} \phi\psi d\underline{x}, \tag{9}$$

respectively, where ϕ, ψ are canonical basis functions of the finite element space. We order the unknowns such that K and M take the following form.

$$K = \begin{pmatrix} K_{11} & 0 & K_{13} \\ 0 & K_{22} & K_{23} \\ K_{13}^T & K_{23}^T & K_{33} \end{pmatrix}, \tag{10}$$

and

$$M = \begin{pmatrix} M_{11} & 0 & M_{13} \\ 0 & M_{22} & M_{23} \\ M_{13}^T & M_{23}^T & M_{33} \end{pmatrix}, \tag{11}$$

where the subscripts $1, 2, 3$ correspond to nodes in the interior of Ω^h, the exterior, and on the boundary, respectively. We split the matrices K_{33} and M_{33} as follows.

$$K_{33} = K_{33}^{(1)} + K_{33}^{(2)}, \tag{12}$$

$$M_{33} = M_{33}^{(1)} + M_{33}^{(2)}. \tag{13}$$

Here $K_{33}^{(1)}$ and $M_{33}^{(1)}$ are constructed from the contributions of Ω^h to the integrals defining the elements of K_{33} and M_{33}, and $K_{33}^{(2)} = K_{33} - K_{33}^{(1)}$ and $M_{33}^{(2)} = M_{33} - M_{33}^{(1)}$ are the corresponding contributions from the exterior. If $K(c)$ is invertible, we use the notation

$$G(c) = \begin{pmatrix} G_{11}(c) & G_{12}(c) & G_{13}(c) \\ G_{12}(c)^T & G_{22}(c) & G_{23}(c) \\ G_{13}(c)^T & G_{23}(c)^T & G_{33}(c) \end{pmatrix} := (K(c))^{-1}, \tag{14}$$

and

$$G := G(0), \qquad G_{ij} := G_{ij}(0). \tag{15}$$

If $K(c)$ is not invertible, $G(c)$ denotes the Moore–Penrose pseudo-inverse of $K(c)$.

We shall use the preconditioned conjugate gradient algorithm. This algorithm can be written in a number of different ways, which are mathematically equivalent, but algorithmically different. We therefore state the form of the algorithm which we shall use: Consider a system of linear equations of the form

$$Q\underline{u} = \underline{b}, \tag{16}$$

where Q is a symmetric, positive semidefinite $n \times n$ matrix. We assume that $\underline{b}$ lies in the range of Q. Let $\tilde{Q}$ be the preconditioner, a symmetric, positive definite $n \times n$ matrix.

Preconditioned Conjugate Gradient Algorithm. Choose $\underline{z}^{(0)} \in R^n$.
$\underline{g}^{(0)} := \underline{b} - Q\tilde{Q}^{-1}\underline{z}^{(0)}$
Replace $\underline{g}^{(0)}$ by its orthogonal projection onto the range of Q.
$\underline{d}^{(0)} := \underline{g}^{(0)}$
$\tilde{\underline{g}}^{(0)} := \tilde{Q}^{-1}\underline{g}^{(0)}$
$\tilde{\underline{d}}^{(0)} := \tilde{\underline{g}}^{(0)}$

For $j = 0, 1, 2, \cdots$:
$\alpha^{(j)} := [\underline{g}^{(j)T}\tilde{\underline{g}}^{(j)}]/[\tilde{\underline{d}}^{(j)T}Q\tilde{\underline{d}}^{(j)}]$
$\underline{z}^{(j+1)} := \underline{z}^{(j)} + \alpha^{(j)}\underline{d}^{(j)}$
$\underline{g}^{(j+1)} := \underline{g}^{(j)} - \alpha^{(j)}Q\tilde{\underline{d}}^{(j)}$
Replace $\underline{g}^{(j+1)}$ by its orthogonal projection onto the range of Q.
$\tilde{\underline{g}}^{(j+1)} := \tilde{Q}^{-1}\underline{g}^{(j+1)}$
$\beta^{(j)} := [\underline{g}^{(j+1)T}\tilde{\underline{g}}^{(j+1)}]/[\underline{g}^{(j)T}\tilde{\underline{g}}^{(j)}]$
$\underline{d}^{(j+1)} := \underline{g}^{(j+1)} + \beta^{(j)}\underline{d}^{(j)}$
$\tilde{\underline{d}}^{(j+1)} := \tilde{\underline{g}}^{(j+1)} + \beta^{(j)}\tilde{\underline{d}}^{(j)}$

The sequence $\underline{u}^{(j)} = \tilde{Q}^{-1}\underline{z}^{(j)}$ converges to a solution of $Q\underline{u} = \underline{b}$. The projections onto the range of Q are without any effect in exact arithmetic. However, in floating point arithmetic, the algorithm may diverge if the kernel of Q is nontrivial and the projections are omitted.

If Q has a nontrivial kernel, $\tilde{Q}$ can have a nontrivial kernel as well, as long as

$$\ker(\tilde{Q}) \subseteq \ker(Q). \tag{17}$$

The inverse of $\tilde{Q}$ should then be replaced by its Moore–Penrose pseudo-inverse.

It was pointed out by Proskurowski and Widlund [17] that the form of the preconditioned conjugate gradient algorithm given above is particularly efficient in the context of iterative imbedding methods, since a large principal minor of the matrix $Q\tilde{Q}^{-1}$ is an identity matrix; see §§4–6. This is only valid for imbedding methods which use an exact solver on the rectangle $(0,1)^2$.

3. Triangulation. In this section, we shall give a very brief discussion of our triangulation algorithm. A more detailed discussion of this algorithm can be found in [4] and [3].

For simplicity, we assume in this section that $\partial\Omega \in C^1$. Modifications needed near corners of $\partial\Omega$ are discussed in [4]. We first cover $(0,1)^2$ by a regular square grid of N-by-N cells. Nodes in this grid that are near $\partial\Omega$ are moved onto the boundary. We have thus two quadrilateral grids: the regular square grid, and a perturbed logically rectangular grid, which is in one-to-one correspondence with the regular grid.

Each of the cells of the perturbed grid is divided into two triangles along one of its diagonals. Away from $\partial\Omega$, the cells are square and they are cut along the diagonal joining the left upper and right lower corners. (This decision is arbitrary.) Near $\partial\Omega$, an attempt is made to make the cuts roughly along $\partial\Omega$, but with the additional requirement that degenerate triangles are not allowed. Figures 1 and 2 illustrate the kind of triangulations generated by our algorithm.

Let ψ_τ denote an affine mapping from the reference triangle

$$\{\underline{x} = (x_1, x_2) \ : \ 0 \le x_1 \le 1, \ \ 0 \le x_2 \le 1 - x_2\} \tag{18}$$

onto a triangle τ. There are several such affine mappings. Let $\hat{\psi}_\tau(0,0)$, $\hat{\psi}_\tau(1,0)$, and $\hat{\psi}_\tau(0,1)$ denote the points in the regular square grid associated with $\psi_\tau(0,0)$, $\psi_\tau(1,0)$, and $\psi_\tau(0,1)$, which are nodes in the perturbed grid. The mapping ψ_τ is made unique by requiring that $\hat{\psi}_\tau(1,0) - \hat{\psi}_\tau(0,0)$, $\hat{\psi}_\tau(0,1) - \hat{\psi}_\tau(0,0)$ be a positively oriented pair of orthogonal vectors.

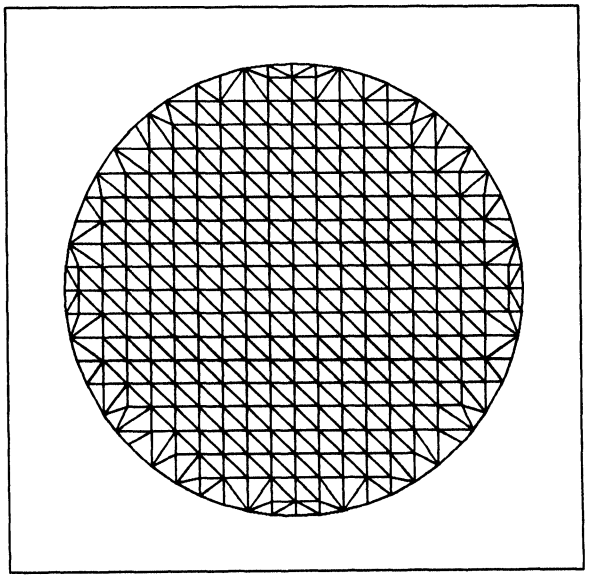

FIG. 1. *Triangulation of* Ω.

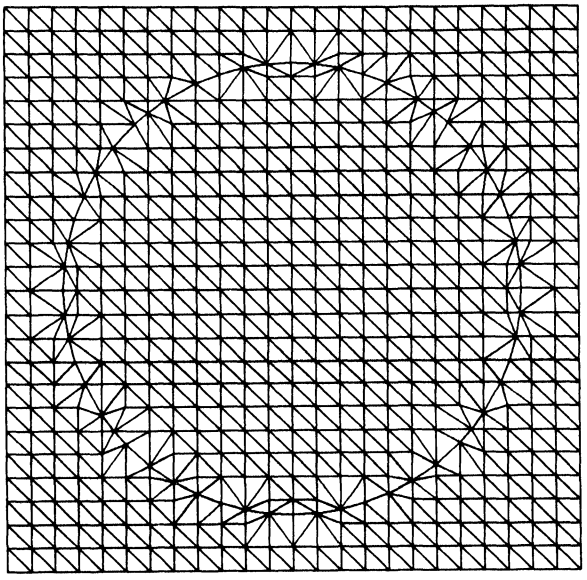

FIG. 2. *Triangulation of* Ω *and its complement.*

Let $D\psi_\tau$ denote the Jacobi matrix of ψ_τ. The spectral condition number of $(D\psi_\tau)^T(D\psi_\tau)$ is a measure of "degeneracy" of τ: The larger it is, the more degenerate is τ. In the present context, this measure of degeneracy is most natural; see [3] or [4]. A proof of the following theorem is also given in [3] and [4].

THEOREM 3.1. *The triangulation algorithm outlined above, and described in detail in* [4], *is guaranteed to generate a triangulation of any arbitrary domain* Ω *with* $\partial\Omega \in C^1$, *such that for all triangles* τ,

$$\text{cond}((D\psi_\tau)^T(D\psi_\tau)) \leq (3+\sqrt{8})^2 \approx 34. \tag{19}$$

This estimate is sharp.

Our triangulation algorithm is an improvement over that of Proskurowski and Widlund [17], which can break down if Ω is not convex.

4. Neumann problems. The finite element discretization of the Neumann problem (1)–(2) leads to the symmetric system

$$\begin{pmatrix} K_{11}(c) & K_{13}(c) \\ K_{13}^T(c) & K_{33}^{(1)}(c) \end{pmatrix} \begin{pmatrix} \underline{x}_1 \\ \underline{x}_3 \end{pmatrix} = \begin{pmatrix} \underline{b}_1 \\ \underline{b}_3 \end{pmatrix}, \tag{20}$$

which is positive semidefinite if $c = 0$, and positive definite if $c > 0$.

As a preconditioner for

$$\begin{pmatrix} K_{11}(c) & K_{13}(c) \\ K_{13}^T(c) & K_{33}^{(1)}(c) \end{pmatrix}, \tag{21}$$

we first consider

$$\left[\begin{pmatrix} I & 0 & 0 \\ 0 & 0 & I \end{pmatrix} G(c) \begin{pmatrix} I & 0 \\ 0 & 0 \\ 0 & I \end{pmatrix} \right]^{-1}. \tag{22}$$

A straightforward computation shows that this matrix equals

$$\begin{pmatrix} K_{11}(c) & K_{13}(c) \\ K_{13}(c)^T & K_{33}^{(1)}(c) + S^{(2)} \end{pmatrix}, \tag{23}$$

where

$$S^{(2)} := K_{33}(c)^{(2)} - K_{23}(c)^T K_{22}(c)^{-1} K_{23}(c). \tag{24}$$

THEOREM 4.1. (21) *and* (22) *are spectrally equivalent, i.e., the quotient of the quadratic forms associated with* (21) *and* (22) *is bounded, on the orthogonal complement of the kernel of* (21), *from below by* $\Lambda_0 > 0$ *and from above by* Λ_1, *with constants* Λ_0 *and* Λ_1 *independent of* h.

Proof. We shall give an outline of the proof for later reference. For details, we refer to [22]. The generalized Rayleigh quotient under consideration is

$$\frac{\begin{pmatrix} \underline{x}_1 \\ \underline{x}_3 \end{pmatrix}^T \begin{pmatrix} K_{11}(c) & K_{13}(c) \\ K_{13}(c)^T & K_{33}^{(1)}(c) + S^{(2)} \end{pmatrix} \begin{pmatrix} \underline{x}_1 \\ \underline{x}_3 \end{pmatrix}}{\begin{pmatrix} \underline{x}_1 \\ \underline{x}_3 \end{pmatrix}^T \begin{pmatrix} K_{11}(c) & K_{13}(c) \\ K_{13}(c)^T & K_{33}^{(1)}(c) \end{pmatrix} \begin{pmatrix} \underline{x}_1 \\ \underline{x}_3 \end{pmatrix}} \tag{25}$$

$$= 1 + \frac{\underline{x}_3^T S^{(2)} \underline{x}_3}{\begin{pmatrix} \underline{x}_1 \\ \underline{x}_3 \end{pmatrix}^T \begin{pmatrix} K_{11}(c) & K_{13}(c) \\ K_{13}(c)^T & K_{33}^{(1)}(c) \end{pmatrix} \begin{pmatrix} \underline{x}_1 \\ \underline{x}_3 \end{pmatrix}} \tag{26}$$

$$(27)\quad = 1 + \frac{\begin{pmatrix} K_{22}(c)^{-1}K_{23}(c)\underline{x}_3 \\ \underline{x}_3 \end{pmatrix}^T \begin{pmatrix} K_{22}(c) & K_{23}(c) \\ K_{23}(c)^T & K_{33}^{(2)}(c) \end{pmatrix} \begin{pmatrix} K_{22}(c)^{-1}K_{23}(c)\underline{x}_3 \\ \underline{x}_3 \end{pmatrix}}{\begin{pmatrix} \underline{x}_1 \\ \underline{x}_3 \end{pmatrix}^T \begin{pmatrix} K_{11}(c) & K_{13}(c) \\ K_{13}(c)^T & K_{33}^{(1)}(c) \end{pmatrix} \begin{pmatrix} \underline{x}_1 \\ \underline{x}_3 \end{pmatrix}}.$$

Clearly, (27) is bounded from below by 1. The second term in (27) can be interpreted as follows. The denominator is the energy (i.e., the Dirichlet integral) of the finite element function on Ω^h with nodal values $(\underline{x}_1, \underline{x}_3)$. The numerator is the energy of the minimum energy extension of that function to a finite element function on $(0,1)^2 - \Omega^h$. We conclude that if any finite element function on Ω^h can be extended to a finite element function on $(0,1)^2$ with an increase in energy by at most a factor of C, then the condition number of the preconditioned matrix is bounded by C. For general conforming finite elements, the existence of an h-independent bound C of this kind has been proved by Widlund [22]. □

Because of the triangles near $\partial\Omega$, $K(c) = K + cM$ does not have the same stencil everywhere, and it cannot be inverted using a fast solver on $(0,1)^2$. In (22), we therefore replace the (pseudo-) inverse $G(c)$ of $K(c)$ by the (pseudo-) inverse of the more convenient, spectrally equivalent 5-point difference operator

$$(28)\qquad \begin{array}{ccc} & -1 & \\ -1 & 4 + ch^2 & -1 \\ & -1 & \end{array}.$$

The spectral equivalence of $K(c)$ and (28) is a consequence of Theorem 1, and provides the motivation for the definition of degeneracy of triangles in §3; see [4].

The domain imbedding method for the problem (1), (2) is the conjugate gradient method for equation (20) using the preconditioner (22), with $K(c)$ replaced by (28). Thus the inverse of the preconditioner is applied to a given finite element function r^h by extending r^h to $(0,1)^2$ with zero values in the nodes outside Ω^h, solving a Poisson problem on $(0,1)^2$ with this extension of r^h as the right-hand side, and restricting the solution of this problem from $(0,1)^2$ to Ω^h. We note that this is an equivalent description of the method given in [17].

Next we consider the choice of boundary conditions for the auxiliary problems on $(0,1)^2$.

THEOREM 4.2. *The constant C in the proof of Theorem* 4.1 *is minimized when homogeneous Neumann boundary conditions are chosen on $\partial(0,1)^2$.*

Proof. The minimum energy extension to $(0,1)^2$ of a finite element function on Ω^h satisfies, in the discrete sense, homogeneous Neumann boundary conditions on $\partial(0,1)^2$. □

We report on numerical results confirming the conclusion of Theorem 4.2 and illustrating the performance of the method. We consider the following test domains.

$$(29)\qquad \{(x_1,x_2) \;:\; [(x_1-0.5)^2 + (x_2-0.5)^2]^{1/2} < 0.4\}$$

$$(30)\qquad \{(x_1,x_2) \;:\; [(x_1-0.5)^2 + (x_2-0.5)^2]^{1/2} \in (0.1, 0.4)\}$$

$$(31)\qquad \{(x_1,x_2) \;:\; [(x_1-0.5)^2 + (x_2-0.5)^2]^{1/2} < 0.4 \;\; x_1 < 0.5 \;\text{ or }\; x_2 < 0.5\}$$

(32) $$(0.2, 0.5)^2 \; - \; [0.475, 0.525] \times [0.2, 0.5].$$

The test problem is

(33) $$-\Delta u \; = \; \sin(x_1 + x_2) \; + \; \text{const. on } \Omega,$$

(34) $$\frac{\partial u}{\partial n} \; = \; 0 \; \text{ on } \partial\Omega,$$

where the constant on the right-hand side is chosen such that the discrete compatibility condition is satisfied. We have found very similar rates of convergence of the iterative method for other right-hand sides. We count the number of calls to the fast solver on $\partial(0,1)^2$ required to reduce the Euclidean norm of the residual by a factor less than 10^{-6}. We present numerical comparisons of the following boundary conditions on $\partial(0,1)^2$:

(i) Periodic in x_1, with period 1 and homogeneous Dirichlet conditions at $x_2 = 0$, $x_2 = 1$.

(ii) Homogeneous Dirichlet conditions on the entire boundary $\partial(0,1)^2$.

(iii) Homogeneous Neumann conditions on the entire boundary $\partial(0,1)^2$.

Table 1 shows our results, which confirm that the Neumann condition on $\partial(0,1)^2$ is the best choice, but they also suggest that the choice of boundary conditions on $\partial(0,1)^2$ is of no great importance.

TABLE 1
Neumann problems for the Poisson equation, exact solver on $\partial(0,1)^2$.

region	h	*number of calls*		
		(i)	(ii)	(iii)
(29)	1/50	16	14	13
	1/100	18	16	15
	1/150	17	15	15
	1/200	16	15	14
	1/250	17	16	15
(30)	1/50	16	15	13
	1/100	18	17	16
	1/150	17	15	15
	1/200	17	15	15
	1/250	18	16	15
(31)	1/50	19	18	16
	1/100	21	20	17
	1/150	20	19	16
	1/200	20	19	16
	1/250	21	20	16
(32)	1/50	23	24	21
	1/100	27	28	25
	1/150	21	21	19
	1/200	18	18	17
	1/250	23	24	21

We now consider the use of inexact solvers for the auxiliary problems on $(0,1)^2$ to increase the efficiency. We use a multigrid V-cycle for (28), with homogeneous Neumann boundary conditions on $\partial(0,1)^2$; see [20]. The ratio of the mesh widths

of consecutive levels is 1/2. Piecewise bilinear interpolation is used to transfer the corrections from a given level to the next finer level, and residuals are transferred from a given level to the next coarser level by using the adjoint of the bilinear interpolation operator. The relaxation method is red-black Gauss–Seidel iteration. Three half sweeps (red-black-red) are carried out before and after each coarse grid correction step.

We find numerically that the spectral radius of the iteration matrix of this cycle is no larger than $\rho = 0.185$ on $n-1$ by $n-1$ grids, where n is a power of 2. By an elementary argument, it follows that the condition number of the domain imbedding method can deteriorate by at most the factor

$$\frac{1+\rho}{1-\rho} = \frac{1.185}{0.815} \approx 1.45; \tag{35}$$

compare [3, §5]. The total amount of work required for the cycle corresponds to five to six Gauss–Seidel iteration steps. Results with this method are shown in Table 2, using (ii) homogeneous Dirichlet conditions on $\partial(0,1)^2$, and (iii) homogeneous Neumann conditions on $\partial(0,1)^2$.

TABLE 2
Neumann problems for the Poisson equation, MG cycle on $\partial(0,1)^2$.

region	h	*number of calls*	
		(ii)	(iii)
(29)	1/32	15	14
	1/64	17	15
	1/128	17	15
	1/256	17	16
(30)	1/32	19	15
	1/64	18	15
	1/128	17	15
	1/256	17	15
(31)	1/32	19	16
	1/64	21	18
	1/128	21	17
	1/256	21	17
(32)	1/32	27	23
	1/64	22	19
	1/128	25	21
	1/256	28	25

We conclude this section with a discussion of the case $c > 0$. If Ω, h, f, and g are fixed, the number of iterations required to reduce the residual by a prescribed factor increases as $c \to 0$, and it is significantly larger for $c > 0, c \approx 0$ than for $c = 0$. This observation will be useful in §6, where exterior Neumann problems for the Helmholtz equation will be used as auxiliary problems in a Dirichlet solver.

If $c = 0$, then $G(c)^{1/2}K(c)G(c)^{1/2}$ is uniformly well-conditioned in the sense that the quotient of the largest and the smallest *nonzero* eigenvalue is bounded uniformly in h. $G(c)^{1/2}K(c)G(c)^{1/2}$ has a simple zero eigenvalue. If $c > 0$, $c \approx 0$, then the condition number of $G(c)^{1/2}K(c)G(c)^{1/2}$ is large, by the continuity of the eigenvalues. There is only one outlying eigenvalue, near zero. For the conjugate gradient method, a small outlying eigenvalue is more harmful than a large one; see [12]. We have found that the method is about 20 percent slower for $c = 0.1$ than for $c = 10$. The speed

of convergence for $c = 10$ is very close to that for $c = 0$. For numerical experiments substantiating these conclusions, see [4].

5. A nonoptimal method for Dirichlet problems. We shall use homogeneous Dirichlet boundary conditions on $\partial(0,1)^2$ in §§5 and 6. (The argument of §4 suggesting the use of Neumann boundary conditions on $\partial(0,1)^2$ is no longer valid here.)

The simplest approach to the Dirichlet problem is to treat it as if it were a Neumann problem, i.e., to solve a problem of the form

$$K_{11}\underline{x}_1 = \underline{b}_1 \tag{36}$$

using the conjugate gradient method with the preconditioner

$$G_{11}^{-1}. \tag{37}$$

THEOREM 5.1. *The preconditioner* (37) *is a nonoptimal preconditioner for* K_{11}, *i.e., the condition number of the preconditioned matrix is not bounded as* $h \to 0$. *It grows linearly with* $1/h$.

A proof of this result is outlined in [4].

Nevertheless, our experiments have lead to the conclusion that this method is more efficient than might be expected. Unlike the method of §6, it requires no modifications on domains that are not grid-aligned. (A domain is grid-aligned if all its boundary nodes lie on the regular square grid, i.e., if the perturbed grid is identical with the regular square grid.) In addition, the auxiliary problems on $(0,1)^2$ can be solved inexactly, while the method of §6 requires the exact solutions.

Table 3 shows some of our numerical results, for the grid-aligned L-shaped domain

$$(0.2,0.8)^2 - [0.5,0.5]^2 \tag{38}$$

as well as the domains (29) and (30), which are not grid-aligned. The test problem is

$$-\Delta u = \sin(x_1 + x_2) \text{ on } \Omega \tag{39}$$

$$u = 0 \text{ on } \partial\Omega. \tag{40}$$

We have also conducted tests which suggest that our numerical results are not significantly influenced by the right-hand side and boundary data.

6. A method which uses exterior Neumann problems. We shall now describe a method for solving Dirichlet problems that makes use of "exterior Neumann problems," more precisely problems of the form

$$-\Delta u = f \text{ on } (0,1)^2 - \overline{\Omega} \tag{41}$$

$$\frac{\partial u}{\partial n} = g \text{ on } \partial\Omega, \tag{42}$$

$$u = 0 \text{ on } \partial(0,1)^2. \tag{43}$$

TABLE 3
Dirichlet problems for the Poisson equation, nonoptimal method.

region	*h*	*number of calls*
(29)	1/50	14
	1/100	22
	1/150	26
	1/200	29
	1/250	32
	1/300	36
(30)	1/50	15
	1/100	23
	1/150	28
	1/200	31
	1/250	35
	1/300	39
(38)	1/50	12
	1/100	17
	1/150	20
	1/200	24
	1/250	25
	1/300	28

The finite element discretization of such a problem leads to a system of linear equation with the matrix

$$K^{(2)} := \begin{pmatrix} K_{22} & K_{23} \\ K_{23}^T & K_{33}^{(2)} \end{pmatrix}. \tag{44}$$

LEMMA 6.1. *The discrete exterior Neumann problem is nonsingular, i.e., the matrix $K^{(2)}$ is invertible if and only if Ω^h is simply connected.*

Proof. The kernel of $K^{(2)}$ consists of the finite element functions on the complement of Ω^h, which are zero on $\partial(0,1)^2$, and which are constant on each triangle in the complement of Ω^h, i.e., constant on each connected component of the complement of Ω^h. All such functions are zero if and only if the complement of Ω^h is connected, i.e., if and only if Ω^h is simply connected. □

At the expense of solving one problem on the square, our problem may be reduced to the form

$$\begin{pmatrix} K_{11} & K_{13} \\ 0 & I \end{pmatrix} \begin{pmatrix} \underline{x}_1 \\ \underline{x}_3 \end{pmatrix} = \begin{pmatrix} \underline{b}_1 \\ \underline{b}_3 \end{pmatrix}. \tag{45}$$

Consider the exterior Neumann problem

$$\begin{pmatrix} K_{22} & K_{23} \\ K_{23}^T & K_{33}^{(2)} \end{pmatrix} \begin{pmatrix} \underline{x}_2 \\ \underline{x}_3 \end{pmatrix} = \begin{pmatrix} K_{23}\underline{b}_3 \\ K_{33}^{(2)}\underline{b}_3 \end{pmatrix}. \tag{46}$$

The solution of this problem is $(\underline{0}, \underline{b}_3)^T$. We compute the solution of (46) using the method of §4, exchanging the roles of Ω^h and its complement. Thus, we solve (46) with the preconditioned conjugate gradient method, using the preconditioner

$$\begin{pmatrix} G_{22} & G_{23} \\ G_{23}^T & G_{33} \end{pmatrix}^{-1}. \tag{47}$$

We then obtain the solution in the form

$$\begin{pmatrix} \underline{0} \\ \underline{b}_3 \end{pmatrix} = \begin{pmatrix} G_{22} & G_{23} \\ G_{23}^T & G_{33} \end{pmatrix} \begin{pmatrix} \underline{z}_2 \\ \underline{z}_3 \end{pmatrix}. \tag{48}$$

Setting

$$\begin{pmatrix} \underline{x}_1 \\ \underline{x}_2 \\ \underline{x}_3 \end{pmatrix} := G \begin{pmatrix} \underline{0} \\ \underline{z}_2 \\ \underline{z}_3 \end{pmatrix}, \tag{49}$$

the solution $(\underline{x}_1, \underline{x}_3)^T$ of (45) is obtained. Table 4 contains numerical results obtained with this method.

TABLE 4
Dirichlet problems for the Poisson equation, method using exterior Poisson Neumann problems.

region	h	*number of calls*
(29)	1/50	10
	1/100	10
	1/150	10
	1/200	10
	1/250	10
	1/300	10
(31)	1/50	12
	1/100	13
	1/150	13
	1/200	13
	1/250	13
	1/300	13
(38)	1/50	12
	1/100	13
	1/150	13
	1/200	13
	1/250	13
	1/300	13

The method as described, so far, fails if Ω^h is multiply connected, a fact that previously apparently has been overlooked. Convergence occurs and is as rapid as on simply connected domains, but the limit is usually not the solution of the problem that we want to solve. The reason is that the system (46) is now singular. $(0, \underline{b}_3)^T$ is still a solution, but there are also others. We shall show that this will necessarily cause the method to fail for some right-hand sides and initial guesses.

Suppose that we use the initial guess

$$\begin{pmatrix} \underline{z}_2^{(0)} \\ \underline{z}_3^{(0)} \end{pmatrix} = \begin{pmatrix} K_{23}\underline{b}_3 \\ K_{33}^{(2)}\underline{b}_3 \end{pmatrix}. \tag{50}$$

This is a most natural choice. It can easily be shown that the conjugate gradient iteration then converges to a limit

$$\begin{pmatrix} \underline{z}_2^\star \\ \underline{z}_3^\star \end{pmatrix} \tag{51}$$

such that the difference

$$\begin{pmatrix} \underline{z}_2^{\star} \\ \underline{z}_3^{\star} \end{pmatrix} - \begin{pmatrix} \underline{z}_2^{(0)} \\ \underline{z}_3^{(0)} \end{pmatrix} \tag{52}$$

is orthogonal to the kernel of $K^{(2)}$ with respect to the Euclidean inner product. Now observe that the initial guess (50) is orthogonal to $\ker(K^{(2)})$, since it lies in the range of $K^{(2)}$. Therefore

$$\begin{pmatrix} \underline{0} \\ \underline{b}_3 \end{pmatrix} = \begin{pmatrix} G_{22} & G_{23} \\ G_{23}^T & G_{33} \end{pmatrix} \begin{pmatrix} \underline{z}_2^{*} \\ \underline{z}_3^{*} \end{pmatrix} \tag{53}$$

can only hold if

$$\begin{pmatrix} G_{22} & G_{23} \\ G_{23}^T & G_{33} \end{pmatrix}^{-1} \begin{pmatrix} \underline{0} \\ \underline{b}_3 \end{pmatrix} \tag{54}$$

is orthogonal to $\ker(K^{(2)})$.

THEOREM 6.2. *The vector* (54) *is orthogonal to* $\ker(K^{(2)})$ *for every* $\underline{b}_3$ *if and only if* Ω^h *is simply connected.*

Proof. We first note that

$$\begin{pmatrix} G_{22} & G_{23} \\ G_{23}^T & G_{33} \end{pmatrix} K^{(2)} = \begin{pmatrix} I & \star \\ 0 & C \end{pmatrix} \tag{55}$$

where the order of the square matrix C equals the number of nodes on the boundary of Ω^h. C is invertible if and only if $K^{(2)}$ is invertible.

The vector (54) is orthogonal to $\ker(K^{(2)})$ if and only if there are vectors $\underline{x}_2$, $\underline{x}_3$ with

$$K^{(2)} \begin{pmatrix} \underline{x}_2 \\ \underline{x}_3 \end{pmatrix} = \begin{pmatrix} G_{22} & G_{23} \\ G_{23}^T & G_{33} \end{pmatrix}^{-1} \begin{pmatrix} \underline{0} \\ \underline{b}_3 \end{pmatrix}. \tag{56}$$

The use of Lemma 1 completes the proof. □

There is a simple way of overcoming the difficulty that we have just described: Replace the exterior Neumann problem (46) by

$$\begin{pmatrix} K_{22} + cI_{22} & K_{23} \\ K_{23}^T & K_{33}^{(2)} + cI_{33} \end{pmatrix} \begin{pmatrix} \underline{x}_2 \\ \underline{x}_3 \end{pmatrix} = \begin{pmatrix} K_{23}\underline{b}_3 \\ (K_{33}^{(2)} + cI_{33})\underline{b}_3 \end{pmatrix}, \tag{57}$$

where $c > 0$ and I_{22}, I_{33} are identity matrices. The preconditioned conjugate gradient method, with the preconditioner (47) can be used.

THEOREM 6.3. *The matrix* (47) *and*

$$\begin{pmatrix} K_{22} + cI_{22} & K_{23} \\ K_{23}^T & K_{33}^{(2)} + cI_{33} \end{pmatrix} \tag{58}$$

are spectrally equivalent.

Proof. The matrix (58) is spectrally equivalent with

$$\begin{pmatrix} K_{22}(c) & K_{23}(c) \\ K_{23}(c)^T & K_{33}^{(2)}(c) \end{pmatrix}, \tag{59}$$

which in turn is spectrally equivalent with

$$\begin{pmatrix} G_{22}(c) & G_{23}(c) \\ G_{23}(c)^T & G_{33}(c) \end{pmatrix}^{-1}. \tag{60}$$

This follows from Theorem 2, with the roles of Ω^h and its complement reversed. The matrix (60) is spectrally equivalent with (47). To prove this, it suffices to show that G and $G(c)$ are spectrally equivalent. This follows from the spectral equivalence of K and $K(c)$, which is an immediate consequence of Poincaré's inequality. □

The discussion at the end of §4 shows that c should not be chosen very small. Experiments suggest that the precise value of c is of little importance. We have always chosen $c = 10$. Table 5 contains numerical results obtained with this method.

TABLE 5
Dirichlet problems for the Poisson equation, method using exterior Helmholtz Neumann problems.

region	h	*number of calls*
(30)	1/50	14
	1/100	14
	1/150	14
	1/200	14
	1/250	14
	1/300	14

7. Summary and discussion. For Neumann problems on relatively simple domains, we have found that the finite element imbedding method is quite efficient. The variant using a multigrid cycle on the rectangle is most efficient, as far as arithmetic is concerned. The only methods we know of that would be more efficient are multigrid methods, applied directly to the problem on the irregular domains; compare, e.g., [7], [12, p. 94], and [20]. We expect that a well-chosen multigrid algorithm would be at least two to three times faster than the method of §5. However, imbedding methods have certain advantages. Their implementation is very much simpler, in particular for higher-order finite elements. A useful feature is the complete separation of issues concerning the geometry of the region from those of the solution of the boundary value problems. In §3, we have outlined a general way of handling the geometry. An additional attractive feature is the delegation of almost all work to a fast Helmholtz solver on a rectangle, which makes it possible to use highly efficient, specialized software, or possibly even special hardware.

As demonstrated in [10] and [15], the imbedding methods can also be implemented relatively easily using very little memory. The basic idea is to exploit the fact that if an appropriate version of the conjugate gradient method is chosen, then during the iteration, the right-hand sides differ from zero only at points within a distance of h from the boundary, and the solution is only required at the same point set. Special solvers have been developed for such purposes and, as demonstrated in [15], they are about as fast as conventional fast Poisson solvers. The solution can also be obtained everywhere, by the end of the iteration, by using a variant of a standard fast Poisson solver which requires only a fraction of the memory normally allotted. In our own experiments we have only used the more conventional approach. We do not know to what extent similar savings of memory could be accomplished by developing a special sparse version of a multigrid method.

The method of §4 can, in a straightforward way, be applied to more general symmetric, positive semidefinite second-order elliptic Neumann problems. Note that

the operator used for the auxiliary problems on $(0,1)^2$ need not be an extension of the operator on Ω.

For Dirichlet problems, the methods we have studied are less efficient. They can also be applied to more general symmetric, positive definite second-order elliptic Dirichlet problems. Note, however, that the method of §6 requires the operator on $(0,1)^2$ to be an extension of the operator on Ω. Since the auxiliary problems on $(0,1)^2$ must be separable in order to allow the use of a fast direct solver, this requirement severely restricts the class of operators for which this method can be applied. A two-stage iterative method has been developed in [10] and it appears to offer real promise of resolving these difficulties. We have no direct experience with that method.

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