FOURIER MATRIX DECOMPOSITION METHODS FOR THE LEAST SQUARES SOLUTION OF SINGULAR NEUMANN AND PERIODIC HERMITE BICUBIC COLLOCATION PROBLEMS

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Abstract. We examine the use of orthogonal spline collocation with piecewise Hermite bicubics for the solution of Poisson's equation on a rectangle subject to either pure Neumann or pure periodic boundary conditions. Emphasis is placed on finding a least squares solution of these singular collocation problems. We apply the technique of matrix decomposition and present explicit formulas for the requisite eigensystems corresponding to two-point Neumann and periodic collocation boundary value problems. The resulting algorithms use fast Fourier transforms for efficiency, and are highly parallel in nature. On an $N \times N$ partition, a fourth order accurate least squares solution is computed at a cost of $O(N^2 \log N)$ operations. We present the results of numerical experiments which demonstrate that our implementations compare very favorably with recent fourth order accurate finite difference and finite element Galerkin codes.

Key Words. Poisson's equation, Neumann and periodic boundary conditions, piecewise Hermite bicubics, orthogonal spline collocation, fast direct solvers, least squares solutions, matrix decomposition algorithms, fast Fourier transforms, parallel implementations.

AMS(MOS) subject classification. 65F05, 65N30, 65N35, 65W05

1. Introduction. The approximate solution of Poisson's equation on a rectangle subject to various boundary conditions (Dirichlet, Neumann, periodic, or mixed) is required in many physical problems, especially in computational fluid dynamics. In the case of the standard five-point finite difference (FD) approximation of order two, Buzbee et al. [9], and Swarztrauber [27] discuss the solution of the corresponding linear systems by Fourier and cyclic reduction methods. The associated software [26], which includes routines implementing deferred corrections to achieve fourth order accuracy, is presented in the package FISHPACK (available through NETLIB at Oak Ridge National Laboratory). Software implementing fast direct algorithms for obtaining fourth order nine-point FD approximations for the Helmholtz problem is discussed by Boisvert in [10,11] and is available as part of ELLPACK [23]. Kaufman

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and Warner [18,19] present a fast algorithm for computing higher-order finite element Galerkin (FEG) solutions of separable elliptic equations. Recently, in [5], fast direct methods have been developed for the solution of linear systems arising when orthogonal spline collocation (OSC) with piecewise Hermite bicubics is applied to the Dirichlet boundary value problem for Poisson's equation on a rectangle.

In this paper, we present algorithms based on piecewise Hermite bicubic OSC for obtaining an approximate solution of Poisson's equation

$$-\Delta u = f(x,y), \qquad (x,y) \in \Omega = (0,1)\times(0,1), \tag{1.1}$$

where u is subject to either the Neumann boundary conditions

$$\begin{aligned} u_x(0,y) = u_x(1,y) = 0, \quad y \in [0,1], \\ u_y(x,0) = u_y(x,1) = 0, \quad x \in [0,1], \end{aligned} \tag{1.2}$$

or the periodic boundary conditions

$$\begin{aligned} u(0,y) = u(1,y), \quad u_x(0,y) = u_x(1,y), \quad y \in [0,1], \\ u(x,0) = u(x,1), \quad u_y(x,0) = u_y(x,1), \quad x \in [0,1]. \end{aligned} \tag{1.3}$$

(The homogeneous boundary conditions in (1.2) are chosen to simplify the presentation, though the discussion can be extended to nonhomogeneous boundary conditions.) Throughout, it is assumed that

$$\int\int_{\Omega} f(x,y)\,dxdy = 0, \tag{1.4}$$

which is a necessary condition for the existence of u satisfying (1.1) subject to either (1.2) or (1.3).

As in FD and FEG approximations, piecewise Hermite bicubic OSC applied to Neumann or periodic boundary value problems for Poisson's equation leads to singular discrete problems. The purpose of this paper is to show how least squares solutions of these singular collocation problems can be obtained by a matrix decomposition (MD) method based on fast Fourier transforms (FFTs). The technique of MD, employed in [5,9,10,11,18,19,27], has its roots in the work of Bickley and McNamee [7], and most notably Lynch, et al. [20], where a procedure is given for solving five-point FD problems for separable partial differential equations. For FD, FEG and OSC discretizations, the technique transforms the corresponding approximation problem with respect to one variable, based on eigensystem information particular

to the discretization method used, thus reducing it to a collection of independent one-dimensional (1-D) discrete problems [4]. Once these 1-D problems are solved, the solution of the original approximation problem is obtained by applying the inverse of the transformation first applied. When Poisson's equation is discretized using 5- or 9-point FDs, FEG with piecewise linear polynomials, or piecewise Hermite bicubic OSC (in the case of Dirichlet boundary conditions), the transformations and their inverses can be efficiently applied using FFTs, and the 1-D problems can be effectively solved since their corresponding matrices are tridiagonal or almost block diagonal [13]. However, the details of the FFTs and the solution of the decoupled 1-D problems depend on the discretization method used. The efficiency of the algorithms which we present in this paper for solving Neumann and periodic problems comes from the ability to provide explicit formulas for the eigensystems corresponding to two-point Neumann and periodic piecewise Hermite cubic collocation problems and the ability to carry out forward and inverse transformations with FFTs. These explicit formulas, like their finite difference counterparts, require that the partition be uniform in the corresponding variable. The partition need not be uniform in the non-transformed variable, although for simplicity of presentation we consider the same uniform partition with respect to both variables.

Since Neumann and periodic collocation problems are singular, our algorithms compute either a least squares solution with a specified value at a given point in Ω or a least squares solution of minimal norm. This is accomplished by first perturbing the right-hand side of the singular collocation problem by an appropriate constant so that a solution of the resulting perturbed problem is guaranteed (although this solution will not be unique). We show that any solution of the perturbed problem is a least squares solution of the original singular problem and that a particular solution of the perturbed problem can be obtained using a modification of the MD method which replaces one decoupled singular 1-D collocation problem with a nonsingular one. Although the idea of perturbing the right-hand side in singular FD problems in order to obtain their least squares solutions is used in [26] (see also [27]) and in [11], no details are given in these papers. It is not explained in [18,19] whether or not the approach of perturbing the right-hand side is used to deal with singular FEG problems. It should be noted that the replacement of one decoupled singular 1-D problem by a nonsingular one is employed in Section 12.4.2 of [25] in the solution of

a singular Neumann FD problem.

A brief outline of the paper is as follows. In Section 2, we introduce the method of OSC with piecewise Hermite bicubics, and establish bounds on the error in the least squares solution of singular Neumann and periodic collocation problems. A description of the MD algorithm which we use to compute a least squares solution of the singular collocation problem is presented in Section 3. The corresponding algorithm for periodic problems is discussed in Section 4, where special methods are also given for solving periodic 1-D collocation problems. Section 5 presents the results of numerical experiments comparing the efficiency of our OSC algorithms with software packages of [11] and [19]. Finally, in a Concluding Remarks section we indicate how the eigensystems presented here can be applied to solve other singular and nonsingular collocation problems corresponding to various types of boundary conditions, and briefly discuss the tremendous potential of OSC-MD algorithms for solving three-dimensional problems on parallel shared or distributed memory machines.

2. Analysis of orthogonal spline collocation for Neumann and periodic problems. We begin by introducing the spaces of piecewise Hermite bicubics and recalling properties of the OSC counterpart of Laplace's operator. In Section 2.2, we use these properties to establish bounds on the error in least squares solution for singular Neumann and periodic collocation problems.

2.1. Piecewise Hermite cubic spaces and some basic results . Let $\{x_k\}_{k=0}^N$ be a uniform partition of $[0,1]$, that is, $x_k = kh$, where $h = 1/N$. Let $\mathcal{S}$ be the space of piecewise Hermite cubics on $[0,1]$ defined by

$$\mathcal{S} = \{v \in C^1[0,1] : v|_{[x_k, x_{k+1}]} \in P_3, k = 0, \ldots, N-1\}, \tag{2.1}$$

where P_3 denotes the set of all polynomials of degree ≤ 3, and let

$$\mathcal{M}_{\mathcal{D}} = \{v \in \mathcal{S} : v(0) = v(1) = 0\}, \tag{2.2}$$

$$\mathcal{M}_{\mathcal{N}} = \{v \in \mathcal{S} : v'(0) = v'(1) = 0\}, \tag{2.3}$$

$$\mathcal{M}_{\mathcal{P}} = \{v \in \mathcal{S} : v(0) = v(1), v'(0) = v'(1)\}. \tag{2.4}$$

Note that the dimension of each of the subspaces $\mathcal{M}_{\mathcal{D}}$, $\mathcal{M}_{\mathcal{N}}$, $\mathcal{M}_{\mathcal{P}}$ is $2N$. For ease of exposition, we will assume that the same partition is used in the x- and y-direction,

although this is not a requirement. In the remainder of this subsection, $\mathcal{M}$ denotes either $\mathcal{M}_{\mathcal{N}} \otimes \mathcal{M}_{\mathcal{N}}$ or $\mathcal{M}_{\mathcal{P}} \otimes \mathcal{M}_{\mathcal{P}}$.

Let the set of Gauss points $\{\xi_m\}_{m=1}^{2N}$ on $[0,1]$ be defined by

$$\xi_{2k+1} = x_k + h\frac{3-\sqrt{3}}{6}, \qquad \xi_{2k+2} = x_k + h\frac{3+\sqrt{3}}{6}, \qquad k = 0, \ldots, N-1.$$

Then we have the following lemma.

LEMMA 2.1. *Given real numbers $\alpha_{m,n}$, $m,n = 1,\ldots,2N$, there exists a unique $v \in \mathcal{M}$ such that*

$$v(\xi_m, \xi_n) = \alpha_{m,n}, \qquad m,n = 1,\ldots,2N.$$

Proof. Modifying the proof of Lemma 5.1 in [21] for $\mathcal{M}_{\mathcal{N}}$ and $\mathcal{M}_{\mathcal{P}}$ in place of $\mathcal{M}_{\mathcal{D}}$, it can be shown that Corollary 5.3 of [21] holds true for $\mathcal{M}_{\mathcal{N}}$ and $\mathcal{M}_{\mathcal{P}}$, and hence our lemma follows easily. □

For functions $v, w \in C(\Omega)$, let $\langle v, w\rangle$ be defined by

$$\langle v, w\rangle = \frac{h^2}{4} \sum_{m,n=1}^{2N} (vw)(\xi_m, \xi_n),$$

where the right hand side is obtained by formally applying the composite Gauss-Legendre quadrature rule

$$\int_0^1 g(x)\,dx \approx \frac{h}{2} \sum_{m=1}^{2N} g(\xi_m) \tag{2.5}$$

to $\int\int_\Omega (vw)(x,y)\,dxdy$ with respect to each variable. It follows from Lemma 2.1 that $\langle\cdot,\cdot\rangle$ is an inner product in $\mathcal{M}$.

Throughout this paper, we will use c to denote a generic positive constant (independent of h).

LEMMA 2.2. *There exists a positive constant c such that*

$$||\nabla v||^2_{L^2(\Omega)} \le c\langle -\Delta v, v\rangle, \qquad v \in \mathcal{M}. \tag{2.6}$$

Proof. Modifying the proof of Theorem 5.5 in [21] for $\mathcal{M}_{\mathcal{N}}$ and $\mathcal{M}_{\mathcal{P}}$ in place of $\mathcal{M}_{\mathcal{D}}$, it can be shown that the second inequality in (2.8) of Corollary 5.6 in [21] holds true for $\mathcal{M}$, that is,

$$||\nabla v||^2_{L^2(\Omega)} \le c|||v|||^2, \qquad v \in \mathcal{M},$$

where

$$|||v|||^2 = \frac{h}{2}\sum_{n=1}^{2N}\int_0^1 \left(\frac{\partial v}{\partial x}\right)^2 (x,\xi_n)\,dx + \frac{h}{2}\sum_{m=1}^{2N}\int_0^1 \left(\frac{\partial v}{\partial y}\right)^2 (\xi_m,y)\,dy.$$

On the other hand, Lemma 3.1 in [16] yields

$$\langle -\Delta v, v\rangle = -\frac{h}{2}\sum_{n=1}^{2N}\frac{h}{2}\sum_{m=1}^{2N}\frac{\partial^2 v}{\partial x^2}(\xi_m,\xi_n)v(\xi_m,\xi_n)$$
$$-\frac{h}{2}\sum_{m=1}^{2N}\frac{h}{2}\sum_{n=1}^{2N}\frac{\partial^2 v}{\partial y^2}(\xi_m,\xi_n)v(\xi_m,\xi_n) \geq |||v|||^2,$$

and hence (2.6) follows. □

Let L_h be an operator from $\mathcal{M}$ into $\mathcal{M}$ defined by

$$(L_h v)(\xi_m,\xi_n) = -\Delta v(\xi_m,\xi_n), \qquad m,n = 1,\ldots,2N. \tag{2.7}$$

THEOREM 2.1. *L_h is a self-adjoint, nonnegative definite operator from $\mathcal{M}$ into $\mathcal{M}$ with respect to $\langle\cdot,\cdot\rangle$. Moreover, $L_h v = 0$ if and only if v is a constant.*

Proof. Using Lemma 3.1 of [16] it easy to verify that

$$\langle -\Delta v, w\rangle = \langle v, -\Delta w\rangle, \qquad v,w \in \mathcal{M},$$

and hence L_h is self-adjoint. The remaining properties of L_h are consequences of (2.6). □

2.2. Neumann and periodic piecewise Hermite bicubic OSC problems. Here we describe and analyze OSC with piecewise Hermite bicubics for finding an approximate solution of Neumann and periodic boundary value problems. With $\mathcal{M}_{\mathcal{N}}$ defined by (2.3), the piecewise Hermite bicubic OSC solution $u_h \in \mathcal{M}_{\mathcal{N}} \otimes \mathcal{M}_{\mathcal{N}}$ of (1.1) and (1.2) is defined by requiring that

$$-\Delta u_h(\xi_m,\xi_n) = f(\xi_m,\xi_n), \qquad m,n = 1,\ldots,2N. \tag{2.8}$$

Similarly, with $\mathcal{M}_{\mathcal{P}}$ defined by (2.4), the piecewise Hermite bicubic OSC solution $u_h \in \mathcal{M}_{\mathcal{P}} \otimes \mathcal{M}_{\mathcal{P}}$ of (1.1) and (1.3) is defined by requiring that (2.8) be satisfied. The Neumann and periodic OSC problems can be reformulated in operator equation form as follows: find $u_h \in \mathcal{M}$ ($\mathcal{M} = \mathcal{M}_{\mathcal{N}} \otimes \mathcal{M}_{\mathcal{N}}$ for the Neumann problem and $\mathcal{M} = \mathcal{M}_{\mathcal{P}} \otimes \mathcal{M}_{\mathcal{P}}$ for the periodic problem) such that

$$L_h u_h = f_h, \tag{2.9}$$

where the operator L_h from $\mathcal{M}$ into $\mathcal{M}$ is defined by (2.7), and $f_h \in \mathcal{M}$ is defined by

$$f_h(\xi_m, \xi_n) = f(\xi_m, \xi_n). \qquad m, n = 1, \ldots, 2N. \tag{2.10}$$

Since $L_h 1 = 0$ and, in general, $\langle f_h, 1\rangle \neq 0$, equation (2.9) may not have a solution in the classical sense. It should be noted that the condition $\langle f_h, 1\rangle = 0$, which is the necessary and sufficient condition for the existence of a solution of (2.9), is the discrete analog of (1.4). Since (2.9) may not have a classical solution, we seek its least squares solution which is $u_h \in \mathcal{M}$ such that

$$\|L_h u_h - f_h\| \leq \|L_h v_h - f_h\|, \qquad v_h \in \mathcal{M}, \tag{2.11}$$

where $\|\cdot\|$ is the norm in $\mathcal{M}$ defined by $\|\cdot\| = \langle \cdot, \cdot \rangle^{1/2}$.

In order to discuss in more detail the least squares solution of (2.9), it is convenient to introduce the operator equation

$$L_h u_h = f_h^*, \tag{2.12}$$

where

$$f_h^* = f_h - \frac{h^2}{4} \sum_{k,l=1}^{2N} f(\xi_k, \xi_l). \tag{2.13}$$

Note that f_h^* is a perturbation of f_h by a constant. Since $\langle f_h^*, 1\rangle = 0$, it follows that equation (2.12) has a solution $u_h \in \mathcal{M}$. Moreover, Theorem 2.1 implies that a general solution of (2.12) is the sum of a particular solution plus a constant. The following results relates a least squares solution of (2.9) to a solution of (2.12).

THEOREM 2.2. *A function $u_h \in \mathcal{M}$ is a least squares solution of (2.9) if and only if u_h is a solution of (2.12). If d and $(\hat{x}, \hat{y}) \in \Omega$ are given and u_h is a solution of (2.12), then*

$$\hat{u}_h(x, y) = u_h(x, y) + d - u_h(\hat{x}, \hat{y}) \tag{2.14}$$

is the unique least squares solution of (2.9) such that $\hat{u}_h(\hat{x}, \hat{y}) = d$. If u_h is a solution of (2.12), then

$$\hat{u}_h = u_h - \langle u_h, 1\rangle \tag{2.15}$$

is the unique least squares solution of (2.9) such that $\|\hat{u}_h\|$ is minimal.

Proof. Assume that u_h is a least squares solution of (2.9). Since (2.12) has a solution, (2.11) gives $||L_h u_h - f_h|| \leq ||f_h^* - f_h||$. Squaring both sides of this inequality, using the self-adjointness of L_h, and $L_h f_h = L_h f_h^*$ (since $L_h 1 = 0$), we obtain $||L_h u_h - f_h^*|| \leq 0$, which obviously implies (2.12).

Assume now that u_h is a solution of (2.12). Writing v_h as $u_h + v_h - u_h$, using again the self-adjointness of L_h and $L_h f_h = L_h f_h^*$, we obtain

$$||L_h v_h - f_h||^2 = ||L_h u_h - f_h||^2 + ||L_h(v_h - u_h)||^2,$$

which implies (2.11).

Since $L_h 1 = 0$, the first part of the theorem implies that $\hat{u}_h$ given by (2.14) is a least squares solution of (2.9). Of course $\hat{u}_h(\hat{x}, \hat{y}) = d$, and uniqueness follows from the first part of the theorem and the second part of Theorem 2.1 which imply that any two least squares solutions of (2.9) differ by a constant.

Let $\hat{u}_h$ be given by (2.15). The first part of the theorem and the second part of Theorem 2.1 imply that if v_h is a least squares solution of (2.9), then $v_h = \hat{u}_h + c$, where c is a constant. Further, since $\langle \hat{u}_h, 1 \rangle = 0$, we have $||v_h||^2 = ||\hat{u}_h||^2 + c^2$, which shows that $\hat{u}_h$ is the unique least squares solution of (2.9) of minimal norm. □

To give a bound on the error in a least squares solution of (2.9) we need the following lemma.

LEMMA 2.3. *If $f \in C^3(\overline{\Omega})$, then*

$$\left| \frac{h^2}{4} \sum_{k,l=1}^{2N} f(\xi_k, \xi_l) \right| \leq ch^3 ||f||_{C^3(\bar{\Omega})}. \tag{2.16}$$

Proof. Inequality (2.16) follows easily from (1.4) and the error bound for the composite Gauss-Legendre quadrature rule (2.5) given, for example, in Section 7.4 of [12]. □

The following result is a counterpart of Theorem 3.2 in [21].

THEOREM 2.3. *Let $u \in C^5(\overline{\Omega})$ be a solution of (1.1) subject to either Neumann or periodic boundary conditions, and let u_h be a least squares solution of the Neumann or periodic piecewise Hermite bicubic OSC problem (2.9). Then*

$$||\nabla(u - u_h)||_{L^2(\Omega)} \leq ch^3 ||u||_{C^5(\bar{\Omega})}. \tag{2.17}$$

Proof. We give the proof for the Neumann boundary value problem, that for the periodic case being similar. Assume that u is a solution of (1.1) subject to (1.2) and

that $u_h \in \mathcal{M} = \mathcal{M}_{\mathcal{N}} \otimes \mathcal{M}_{\mathcal{N}}$ is a least squares solution of (2.9). Let $u_I \in \mathcal{M}$ be the piecewise Hermite bicubic interpolant to u. Then, we obtain

$$||\nabla(u - u_I)||_{L^2(\Omega)} \leq ch^3 ||u||_{C^4(\bar{\Omega})}, \tag{2.18}$$

(see [8], for example). Consider $v = u_I - u_h$. It follows from the first part of Theorem 2.2, (2.9), (2.10), (1.1), and (2.16), that

$$\langle -\Delta v, v\rangle = \langle \Delta(u - u_I) + \frac{h^2}{4} \sum_{k,l=1}^{2N} f(\xi_k, \xi_l), v\rangle \leq ch^3 ||u||_{C^5(\bar{\Omega})} \langle v, v\rangle^{1/2}, \tag{2.19}$$

since

$$|\Delta(u - u_I)(\xi_m, \xi_n)| \leq ch^3 ||u||_{C^5(\bar{\Omega})}, \qquad m, n = 1, \ldots, 2N,$$

(cf. Lemma 4.2 in [3]). If necessary, u_h can be changed by adding a constant, which has no effect on (2.17), so that

$$\langle v, v\rangle^{1/2} \leq c\langle -\Delta v, v\rangle^{1/2}. \tag{2.20}$$

Thus, by (2.19), (2.20) and (2.6), we have

$$||\nabla(u_I - u_h)||_{L^2(\Omega)} \leq ch^3 ||u||_{C^5(\bar{\Omega})}. \tag{2.21}$$

Hence, (2.17) follows from (2.18), (2.21), and the triangle inequality. □

3. The OSC matrix decomposition algorithm for Neumann problems. In this section, we describe the linear system arising in the singular Neumann collocation problem (2.9) and give details of the associated MD algorithm for obtaining its least squares solution. We specifically address the singularity of the Neumann collocation problem, which manifests itself in the singularity of one of the decoupled 1-D collocation problems.

Let $\{\phi_n\}_{n=1}^{2N}$ be a set of Hermite basis functions for $\mathcal{M}_{\mathcal{N}}$ defined in the following way: for $k = 0, \ldots, N$,

$$\begin{aligned} \phi_n(x_k) = \delta_{n,k+1}, \qquad \phi_n'(x_k) = 0, \qquad n = 1, \ldots, N+1, \\ \phi_{N+n}(x_k) = 0, \qquad \phi_{N+n}'(x_k) = h^{-1}\delta_{n,k+1}, \qquad n = 2, \ldots, N, \end{aligned} \tag{3.1}$$

where $\delta_{n,k}$ is the Kronecker delta, and let $\{\psi_n\}_{n=1}^{2N}$ represent the set of basis functions for $\mathcal{M}_{\mathcal{N}}$ obtained by rearranging $\{\phi_n\}_{n=1}^{2N}$ as follows

$$\psi_1 = \phi_1, \qquad \psi_{2(k-1)} = \phi_k, \quad \psi_{2k-1} = \phi_{N+k}, \quad k = 2, \ldots, N, \qquad \psi_{2N} = \phi_{N+1}. \tag{3.2}$$

Assume that

$$u_h(x,y) = \sum_{m,n=1}^{2N} u_{m,n}\phi_m(x)\psi_n(y) \tag{3.3}$$

is a solution of the Neumann collocation problem (2.12), and take

$$\mathbf{u} = [\mathbf{u}_1, \ldots, \mathbf{u}_{2N}]^T, \qquad \mathbf{u}_m = [u_{m,1}, \ldots, u_{m,2N}], \tag{3.4}$$

$$\mathbf{f}^* = [\mathbf{f}_1^*, \ldots, \mathbf{f}_{2N}^*]^T, \qquad \mathbf{f}_m^* = [f_{m,1}^*, \ldots, f_{m,2N}^*], \tag{3.5}$$

where

$$f_{m,n}^* = f(\xi_m, \xi_n) - \frac{h^2}{4} \sum_{k,l=1}^{2N} f(\xi_k, \xi_l). \tag{3.6}$$

Then $\mathbf{u}$ satisfies

$$(A_x \otimes B_y + B_x \otimes A_y)\mathbf{u} = \mathbf{f}^*, \tag{3.7}$$

where the matrices A_x and B_x are defined by

$$\begin{aligned} A_x &= (a_{m,n})_{m,n=1}^{2N}, \qquad a_{m,n} = -\phi_n''(\xi_m), \\ B_x &= (b_{m,n})_{m,n=1}^{2N}, \qquad b_{m,n} = \phi_n(\xi_m), \end{aligned} \tag{3.8}$$

and A_y and B_y are defined by

$$\begin{aligned} A_y &= (a_{m,n})_{m,n=1}^{2N}, \qquad a_{m,n} = -\psi_n''(\xi_m), \\ B_y &= (b_{m,n})_{m,n=1}^{2N}, \qquad b_{m,n} = \psi_n(\xi_m). \end{aligned} \tag{3.9}$$

Explicit formulas are derived in [1] for a diagonal matrix $\Lambda_{\mathcal{N}} = \mathrm{diag}(\lambda_j^{\mathcal{N}})_{j=1}^{2N}$ and nonsingular matrix $Z_{\mathcal{N}}$ which satisfy the equations

$$Z_{\mathcal{N}}^T B_x^T A_x Z_{\mathcal{N}} = \Lambda_{\mathcal{N}}, \qquad Z_{\mathcal{N}}^T B_x^T B_x Z_{\mathcal{N}} = I, \tag{3.10}$$

where I is the identity matrix of order $2N$. See (A.1), (A.3), and (A.4) in Appendix A for a statement of these formulas and equations. It follows from (3.10) and properties of the tensor product that

$$(Z_{\mathcal{N}}^T B_x^T \otimes I)(A_x \otimes B_y + B_x \otimes A_y)(Z_{\mathcal{N}} \otimes I) = \Lambda_{\mathcal{N}} \otimes B_y + I \otimes A_y. \tag{3.11}$$

Equations (3.7) and (3.11) show that, if the vectors $\mathbf{g}$ and $\mathbf{v}$ are defined by

$$\mathbf{g} = (Z_{\mathcal{N}}^T B_x^T \otimes I)\mathbf{f}^*, \qquad \mathbf{v} = (Z_{\mathcal{N}} \otimes I)^{-1}\mathbf{u},$$

then

$$(\Lambda_{\mathcal{N}} \otimes B_y + I \otimes A_y)\mathbf{v} = \mathbf{g}. \tag{3.12}$$

If we set

$$\mathbf{v} = [\mathbf{v}_1, \ldots, \mathbf{v}_{2N}]^T, \qquad \mathbf{v}_m = [v_{m,1}, \ldots, v_{m,2N}],$$

$$\mathbf{g} = [\mathbf{g}_1, \ldots, \mathbf{g}_{2N}]^T, \qquad \mathbf{g}_m = [g_{m,1}, \ldots, g_{m,2N}],$$

then (3.12) can be written as

$$A_y \mathbf{v}_1 = \mathbf{g}_1, \tag{3.13}$$

since $\lambda_1 = 0$, and

$$(A_y + \lambda_j^{\mathcal{N}} B_y)\mathbf{v}_j = \mathbf{g}_j, \qquad j = 2, \ldots, 2N. \tag{3.14}$$

It should be noted that while the matrix A_y is singular, the matrices $A_y + \lambda_j^{\mathcal{N}} B_y$, $j = 2, \ldots, 2N$, are nonsingular since $A_y B_y^{-1}$ is a symmetric nonnegative matrix and since by (A.2), $\lambda_j^{\mathcal{N}} > 0$ for $j = 2, \ldots, 2N$. The singular linear system (3.13) is the matrix-vector form of the singular 1-D collocation problem

$$-v''(\xi_m) = g(\xi_m), \qquad m = 1, \ldots, 2N, \qquad v \in \mathcal{M}_{\mathcal{N}}, \tag{3.15}$$

where $g(\xi_m) = \mathbf{g}_{1,m}$. Since (3.13) has a solution, it follows that (3.15) also has a solution. Further, if v is a solution of (3.15), then so is v plus a constant. Hence, there is a solution v of (3.15) such that

$$-v''(\xi_m) = g(\xi_m), \quad m = 1, \ldots, 2N, \quad v \in \mathcal{S}, \quad v'(0) = 0, \quad v(1) = 0. \tag{3.16}$$

Obviously, (3.16) is a nonsingular problem, since a Dirichlet, rather than a Neumann, boundary condition is imposed at the right-hand end point of $[0, 1]$. Corresponding to the solution v of (3.16), there are $\mathbf{v}_1$ and u_h which are solutions of (3.13) and (2.12), respectively. Hence, based on Theorem 2.2, we arrive at the following MD algorithm for computing the least squares solution $\hat{u}_h$ of (2.9) such that $\hat{u}_h(\hat{x}, \hat{y}) = d$ or such that $||\hat{u}_h||$ is minimal.

OSC-MD Neumann Algorithm

1. Compute $\mathbf{g} = (Z_N^T B_x^T \otimes I)\mathbf{f}^*$, where $\mathbf{f}^*$ is given by (3.5) and (3.6).
2. Solve (3.16) and thus obtain the corresponding $\mathbf{v}_1$ of (3.13).
3. Solve the linear systems (3.14).
4. Compute $\mathbf{u} = (Z_N \otimes I)\mathbf{v}$.
5. Compute $\hat{u}_h$ using either (2.14) or (2.15).

Since there are at most four nonzero elements in each column of the matrix B_x, the matrix-vector multiplications involving the matrix B_x^T in Step 1 require, in total, $O(N^2)$ arithmetic operations. It follows from (A.3) that FFT routines can be used to perform multiplications by the matrix Z_N^T in Step 1, and Z_N in Step 4. The corresponding cost of each of these steps is $O(N^2 \log N)$. Each vector $\mathbf{v}_j$, $j = 1, \ldots, 2N$, in Step 2 and 3 can be effectively computed by the package COLROW [14], [15], with a cost of $O(N)$. Thus the total cost of the OSC-MD Neumann Algorithm is $O(N^2 \log N)$ operations.

Suppose that the OSC-MD Neumann Algorithm is carried out for

$$\mathbf{f} = [\mathbf{f}_1, \ldots, \mathbf{f}_{2N}]^T, \quad \mathbf{f}_m = [f_{m,1}, \ldots, f_{m,2N}], \quad f_{m,n} = f(\xi_m, \xi_n) \tag{3.17}$$

in place of $\mathbf{f}^*$ in Step 1, thus yielding $\tilde{u}_h$ in place of $\hat{u}_h$. Although, in general, $\tilde{u}_h$ will be different from $\hat{u}_h$, it can be shown, using (2.16), that

$$||\nabla(\tilde{u}_h - \hat{u}_h)||_{L^2(\Omega)} \leq ch^3 ||f||_{C^3(\bar{\Omega})},$$

which along with Theorem 2.3 gives

$$||\nabla(u - \tilde{u}_h)||_{L^2(\Omega)} \leq ch^3 ||u||_{C^5(\bar{\Omega})}. \tag{3.18}$$

4. The OSC matrix decomposition algorithm for periodic problems. We describe in this section the periodic analog of the OSC-MD Neumann algorithm of the previous section, and an alternate approach for finding a least squares solution of periodic collocation problem (2.9).

4.1. The OSC-MD Periodic Algorithm. The basis functions $\{\phi_n\}_{n=1}^{2N}$ for $\mathcal{M}_p$ are defined in the following way: for $k = 0, \ldots, N$,

$$
\begin{aligned}
&\phi_1(0) = \phi_1(1) = 1, \quad \phi_1(x_k) = 0, \quad k \neq 0, N, \quad \phi_1'(x_k) = 0, \\
&\phi_n(x_k) = \delta_{n,k+1}, \quad \phi_n'(x_k) = 0, \quad n = 2, \ldots, N, \\
&\phi_{N+1}'(0) = \phi_{N+1}'(1) = h^{-1}, \quad \phi_{N+1}'(x_k) = 0, \quad k \neq 0, N, \quad \phi_{N+1}(x_k) = 0, \\
&\phi_{N+n}(x_k) = 0, \quad \phi_{N+n}'(x_k) = h^{-1}\delta_{n,k+1}, \quad n = 2, \ldots, N.
\end{aligned} \tag{4.1}
$$

The basis functions $\{\psi_n\}_{n=1}^{2N}$ for $\mathcal{M}_p$ are obtained by reordering of $\{\phi_n\}_{n=1}^{2N}$ so that

$$
\psi_{2k-1} = \phi_k, \quad \psi_{2k} = \phi_{N+k}, \quad k = 1, \ldots, N. \tag{4.2}
$$

Assume that u_h given as in (3.3) is a solution of the periodic problem (2.12). Then $\mathbf{u}$, as defined by (3.4), satisfies (3.7), where the matrices A_x, B_x and A_y, B_y are given by (3.8) and (3.9) but now with the basis functions $\{\phi_n\}_{n=1}^{2N}$ and $\{\psi_n\}_{n=1}^{2n}$ defined by (4.1) and (4.2). As in the Neumann case, formulas exist for a diagonal matrix $\Lambda_p = \mathrm{diag}(\lambda_j^p)_{j=1}^{2N}$ and nonsingular matrix Z_p such that

$$
Z_p^T B_x^T A_x Z_p = \Lambda_p, \quad Z_p^T B_x^T B_x Z_p = I.
$$

These formulas and equations are derived in [1] and presented in (A.5), (A.6), and (A.7) in the Appendix of this paper.

Substituting A_x, B_x, A_y, B_y, Z_p and λ_j^p of this section for their Neumann counterparts in the OSC-MD Neumann Algorithm we obtain the following algorithm for computing a least squares solution of the periodic collocation problem (2.9), which we include for completeness.

OSC-MD Periodic Algorithm

1. Compute $\mathbf{g} = (Z_p^T B_x^T \otimes I)\mathbf{f}^*$, where $\mathbf{f}^*$ is given by (3.5) and (3.6).
2. Solve (3.16) and thus obtain the corresponding $\mathbf{v}_1$ of (3.13).
3. Solve the linear systems (3.14) with λ_j^p in place of λ_j^N.
4. Compute $\mathbf{u} = (Z_p \otimes I)\mathbf{v}$.
5. Compute $\hat{u}_h$ using either (2.14) or (2.15).

The package COLROW cannot be used directly to carry out Steps 2 and 3 in the OSC-MD Periodic Algorithm since the matrices A_y and B_y contain not only almost diagonal blocks, but also a block in the lower left corner (thus, they do not possess

a true almost block diagonal structure). However, we will show in this section that solving such linear systems can be reduced to the solution of two almost block diagonal linear systems corresponding to 1-D collocation Dirichlet and Neumann problems. To this end, we note that Steps 2 and 3 in the periodic case are equivalent to finding v_j, $j = 1, \ldots, 2N$, such that

$$-v_j''(\xi_m) + \lambda_j^{\mathcal{P}} v_j(\xi_m) = g_j(\xi_m), \qquad m = 1, \ldots, 2N, \qquad v_j \in \mathcal{M}_{\mathcal{P}}, \tag{4.3}$$

where $g_j(\xi_m) = g_{j,m}$. For $j = 2, \ldots, 2N$, we seek v_j in the form

$$v_j = v_j^{(1)} + \gamma_j v_j^{(2)}, \tag{4.4}$$

where the parameter γ_j is to be determined, and where $v_j^{(i)}$, $i = 1, 2$, are such that

$$-[v_j^{(1)}]''(\xi_m) + \lambda_j^{\mathcal{P}} v_j^{(1)}(\xi_m) = g_j(\xi_m), \qquad m = 1, \ldots, 2N, \qquad v_j^{(1)} \in \mathcal{M}_{\mathcal{D}}, \tag{4.5}$$

$$\begin{gathered} -[v_j^{(2)}]''(\xi_m) + \lambda_j^{\mathcal{P}} v_j^{(2)}(\xi_m) = 0, \qquad m = 1, \ldots, 2N, \qquad v_j^{(2)} \in \mathcal{S}, \\ v_j^{(1)}(0) = v_j^{(1)}(1) = 1. \end{gathered} \tag{4.6}$$

It is easy to verify that, for any γ_j, v_j satisfies (4.3) and $v_j(0) = v_j(1)$. To satisfy the condition $v_j'(0) = v_j'(1)$, γ_j should be selected according to the formula

$$\gamma_j = \frac{[v_j^{(1)}]'(1) - [v_j^{(1)}]'(0)}{[v_j^{(2)}]'(0) - [v_j^{(2)}]'(1)}. \tag{4.7}$$

Since $\lambda_1^{\mathcal{P}} = 0$, (4.3) for $j = 1$ reduces to the singular 1-D collocation problem

$$-v_1''(\xi_m) = g_1(\xi_m), \qquad m = 1, \ldots, 2N, \qquad v_1 \in \mathcal{M}_{\mathcal{P}}; \tag{4.8}$$

cf. (3.15). In the OSC-MD Periodic Algorithm, (4.8) is replaced by the nonsingular 1-D collocation problem

$$-v_1''(\xi_m) = g_1(\xi_m), \qquad m = 1, \ldots, 2N, \qquad v_1 \in \mathcal{M}_{\mathcal{D}}; \tag{4.9}$$

cf. (3.16).

For even N, the functions v_j, $j = 1, \ldots, 2N$, satisfying (4.3) can be also obtained using an approach based on the following observation: if for $j = 1, \ldots, 2N$,

$$v_j^{\mathcal{D}}, v_j^{\mathcal{N}} \in \{v \in C^1[0, 1/2] : v|_{[x_k, x_{k+1}]} \in P_3, k = 0, \ldots, N/2 - 1\},$$

are such that

$$
\begin{aligned}
-[v_j^p]''(\xi_m) + \lambda_j^p v_j^p(\xi_m) &= g_j(\xi_m) - g_j(1-\xi_m), \quad m = 1, \ldots, N, \\
v_j^p(0) = v_j^p(1/2) &= 0,
\end{aligned} \tag{4.10}
$$

$$
\begin{aligned}
-[v_j^{\mathcal{N}}]''(\xi_m) + \lambda_j^p v_j^{\mathcal{N}}(\xi_m) &= g_j(\xi_m) + g_j(1-\xi_m), \quad m = 1, \ldots, N, \\
[v_j^{\mathcal{N}}]'(0) = [v_j^{\mathcal{N}}]'(1/2) &= 0,
\end{aligned} \tag{4.11}
$$

then v_j, defined by

$$
\begin{aligned}
v_j(x) &= [v_j^p(x) + v_j^{\mathcal{N}}(x)]/2, \qquad x \in [0, 1/2], \\
v_j(x) &= [v_j^{\mathcal{N}}(1-x) - v_j^p(1-x)]/2, \qquad x \in [1/2, 1],
\end{aligned} \tag{4.12}
$$

satisfies (4.3). Since $\lambda_1^p = 0$, (4.11) for $j = 1$ reduces to the singular 1-D collocation problem

$$
\begin{aligned}
-[v_1^{\mathcal{N}}]''(\xi_m) &= g_1(\xi_m) + g_1(1-\xi_m), \quad m = 1, \ldots, N, \\
[v_1^{\mathcal{N}}]'(0) = [v_1^{\mathcal{N}}]'(1/2) &= 0;
\end{aligned} \tag{4.13}
$$

cf. (3.15). The problem (4.13) is replaced in the OSC-MD Periodic Algorithm by the nonsingular 1-D collocation problem

$$
\begin{aligned}
-[v_1^{\mathcal{N}}]''(\xi_m) &= g_1(\xi_m) + g_1(1-\xi_m), \quad m = 1, \ldots, N, \\
[v_1^{\mathcal{N}}]'(0) = 0, \qquad [v_1^{\mathcal{N}}](1/2) &= 0;
\end{aligned} \tag{4.14}
$$

cf. (3.16).

Problems (4.5), (4.6), $j = 2, \ldots, 2N$, and (4.9), as well as problems (4.10), (4.11), $j = 2, \ldots, 2N$, and (4.14) can be solved using the package COLROW. For even N, the cost of solving (4.10), (4.11), $j = 2, \ldots, 2N$, and (4.14) is about half of that for solving (4.5), (4.6), $j = 2, \ldots, 2N$, and (4.9), since in the second approach we solve 1-D collocation problems on the interval $[0, 1/2]$ rather than on $[0, 1]$. However, the approach based on solving (4.5), (4.6), $j = 2, \ldots, 2N$, and (4.9) is applicable for odd as well as even N, and also for the case when the partition with respect to y is nonuniform. It should be noted that a similar approach is employed in Section 2.2.2 of [24] for the solution of periodic FD problems. Since FFTs can be used again in Steps 1 and 4 of the OSC-MD Periodic Algorithm (see (A.6)), its total cost is $O(N^2 \log N)$ operations.

It should be noted that applying the OSC-MD Periodic Algorithm with $\mathbf{f}$ of (3.17) in place of $\mathbf{f}^*$ in Step 1 yields a solution $\tilde{u}_h$ which satisfies (3.18).

4.2. An alternate approach for periodic problems. Assume that N is even and set $N' = N/2$. Let u_h be a periodic collocation solution of (2.12) and consider

$$v(x,y) = u_h(x,y) - u_h(1-x,y), \qquad (x,y) \in [0,1/2] \times [0,1], \tag{4.15}$$

$$w(x,y) = u_h(x,y) + u_h(1-x,y), \qquad (x,y) \in [0,1/2] \times [0,1]. \tag{4.16}$$

Clearly, if v, w were known, then we would also know u_h since

$$u_h(x,y) = [v(x,y) + w(x,y)]/2, \qquad (x,y) \in [0,1/2] \times [0,1],$$

$$u_h(x,y) = [w(1-x,y) - v(1-x,y)]/2, \qquad (x,y) \in [1/2,1] \times [0,1].$$

Let $\mathcal{M}'_{\mathcal{D}}$, $\mathcal{M}'_{\mathcal{N}}$, and $\mathcal{M}'_{\mathcal{P}}$ be defined by (2.2), (2.3), and (2.4), respectively, where 1 is replaced by $1/2$, and $\mathcal{S}$ is defined by (2.1) with $[0,1]$ and N replaced by $[0,1/2]$ and N', respectively. It follows from (4.15) and (2.12) that $v \in \mathcal{M}'_{\mathcal{D}} \otimes \mathcal{M}_{\mathcal{P}}$ and

$$-\Delta v(\xi_m,\xi_n) = f_h^*(\xi_m,\xi_n) - f_h^*(1-\xi_m,\xi_n), \qquad m = 1,\ldots,N, n = 1,\ldots,M.$$

Similarly, $w \in \mathcal{M}'_{\mathcal{N}} \otimes \mathcal{M}_{\mathcal{P}}$ and

$$-\Delta w(\xi_m,\xi_n) = f_h^*(\xi_m,\xi_n) + f_h^*(1-\xi_m,\xi_n), \qquad m = 1,\ldots,N, n = 1,\ldots,M.$$

Further, if we set

$$v^{\pm}(x,y) = v(x,y) \pm v(x,1-y), \qquad (x,y) \in [0,1/2] \times [0,1/2], \tag{4.17}$$

$$w^{\pm}(x,y) = w(x,y) \pm w(x,1-y), \qquad (x,y) \in [0,1/2] \times [0,1/2], \tag{4.18}$$

then $v^- \in \mathcal{M}'_{\mathcal{D}} \otimes \mathcal{M}'_{\mathcal{D}}$, and

$$-\Delta v^-(\xi_m,\xi_n) = g^{(1)}(\xi_m,\xi_n), \qquad m,n = 1,\ldots,N, \tag{4.19}$$

where, by (2.13) and (2.10),

$$g^{(1)}(\xi_m,\xi_n) = f(\xi_m,\xi_n) - f(1-\xi_m,\xi_n) - f(\xi_m,1-\xi_n) + f(1-\xi_m,1-\xi_n).$$

Similarly, $v^+ \in \mathcal{M}'_{\mathcal{D}} \otimes \mathcal{M}'_{\mathcal{N}}$,

$$-\Delta v^+(\xi_m,\xi_n) = g^{(2)}(\xi_m,\xi_n), \qquad m,n = 1,\ldots,N, \tag{4.20}$$

where

$$g^{(2)}(\xi_m,\xi_n) = f(\xi_m,\xi_n) - f(1-\xi_m,\xi_n) + f(\xi_m,1-\xi_n) - f(1-\xi_m,1-\xi_n),$$

and $w^- \in \mathcal{M}'_{\mathcal{N}} \otimes \mathcal{M}'_{\mathcal{D}}$,

$$-\Delta w^-(\xi_m,\xi_n) = g^{(3)}(\xi_m,\xi_n), \qquad m,n = 1,\ldots,N, \tag{4.21}$$

where

$$g^{(3)}(\xi_m,\xi_n) = f(\xi_m,\xi_n) + f(1-\xi_m,\xi_n) - f(\xi_m,1-\xi_n) - f(1-\xi_m,1-\xi_n),$$

and $w^+ \in \mathcal{M}'_{\mathcal{N}} \otimes \mathcal{M}'_{\mathcal{N}}$,

$$-\Delta w^+(\xi_m,\xi_n) = g^{(4)}(\xi_m,\xi_n), \qquad m,n = 1,\ldots,N, \tag{4.22}$$

where

$$\begin{aligned} g^{(4)}(\xi_m,\xi_n) \quad = \quad & f(\xi_m,\xi_n) + f(1-\xi_m,\xi_n) + f(\xi_m,1-\xi_n) \\ & + f(1-\xi_m,1-\xi_n) - h^2 \sum_{k,l=1}^{2N} f(\xi_k,\xi_l). \end{aligned}$$

Thus finding the periodic collocation solution of (2.12) is reduced to solving four independent collocation problems (4.19)–(4.22). The nonsingular problem (4.19) can be solved by the MD algorithm of [5], while the nonsingular problems (4.20) and (4.21) can be solved by the MD algorithm of [1] (see also [17]). A solution of the singular problem (4.22) can be obtained by performing the first three steps of the OSC-MD Neumann Algorithm of this paper. It follows from (4.15)–(4.18) that the solution u_h of the periodic problem (2.12) is given by

$$u_h(x,y) = \frac{1}{4} \begin{cases} v^-(x,y) + v^+(x,y) + w^-(x,y) + w^+(x,y), \\ \qquad\qquad (x,y) \in [0,1/2]\times[0,1/2], \\ v^+(x,1-y) - v^-(x,1-y) + w^+(x,1-y) - w^-(x,1-y), \\ \qquad\qquad (x,y) \in [0,1/2]\times[1/2,1], \\ w^-(1-x,y) + w^+(1-x,y) - v^-(1-x,y) - v^+(1-x,y), \\ \qquad\qquad (x,y) \in [1/2,1]\times[0,1/2], \\ v^-(1-x,1-y) - v^+(1-x,1-y) \\ \qquad -w^-(1-x,1-y) + w^+(1-x,1-y), \\ \qquad\qquad (x,y) \in [1/2,1]\times[1/2,1]. \end{cases} \tag{4.23}$$

Thus, using (4.23), the periodic least squares solution of (2.9) with a specified value at $(\hat{x},\hat{y}) \in \Omega$ or the least squares solution of minimal norm can be obtained from either (2.14) or (2.15).

5. Numerical results. In this section, we compare the accuracy and efficiency of our algorithms with the package SERRG2 [19], which implements an MD algorithm for the higher-order FEG solution of separable elliptic problems, and HFFT2 [11], which implements an FFT MD algorithm for the fourth order 9-point FD solution of the Helmholtz equation. SERRG2 was obtained as ALG685 in the TOMS directory of NETLIB (netlib@ornl.gov), and the latest version of HFFT2 was obtained directly from its author in a private communication. The SERRG2 package provides the most useful comparison because it gives an approximate solution over the entire domain, unlike FD codes, which provide a solution only at the nodal points of the partition. Further, SERRG2 provides derivative approximations which are unavailable with the HFFT2 package. We use SERRG2 with the space of piecewise bicubic splines rather than Hermite bicubics, since the former choice appears to be more efficient. With this choice of approximation space for SERRG2, all of the methods employed in this study produce approximate solutions which are fourth order accurate.

In each of our test problems, we solve Poisson's equation on the unit square with the right-hand side f chosen so that the equation is satisfied for the specified true solution, $u(x, y)$. The problems, which are summarized in Table 5.1, were run on a sequence of uniform $N \times N$ partitions with $N = 2^i$, where $i = 3, ..., 8$. All of the programs were run on a SUN 4 workstation, using the f77 compiler with the -O flag for program optimization. The compiler flag -r8 was used to obtain a double precision version of the HFFT2 code.

TABLE 5.1

Test problems

True solution	Boundary conditions
(1) $u(x, y) = e^{\cos \pi x \cos \pi y}$	Neumann
(2) $u(x, y) = \cos 4\pi x \cos 4\pi y$	Neumann
(3) $u(x, y) = e^{\sin 2\pi x \sin 2\pi y}$	periodic
(4) $u(x, y) = \cos 4\pi y + \sin 4\pi (x - y)$	periodic

For each problem, we present two graphs of experimental data, each plotting total program execution time versus maximum absolute error in the approximations. The

first of each pair of plots (Figs. 5.1, 5.3, 5.5, 5.7) shows errors in the approximate solution for each algorithm, while the second (Figs. 5.2, 5.4, 5.6, 5.8) shows errors in the approximate derivatives calculated by the OSC-MD and SERRG2 packages. The OSC-MD and SERRG2 derivative results include approximations to the first derivatives. We also report the errors in the mixed second derivative approximations obtained by OSC-MD, since values of this derivative at the nodes are part of the code output. The errors for OSC-MD and SERRG2 were calculated both in a global sense (as the maximum absolute error on a 101×101 uniform partition, including the boundary), and at the nodal points of the partition. For HFFT2, of course, the errors were calculated only at the nodes. Since superconvergent derivative approximations were observed at the partition nodes in the case of OSC-MD, we present the nodal information in the graphs (as "OSC-MD-nodal"). Nodal and global results for SERRG2 were virtually identical, therefore only the latter set of data is shown. For both SERRG2 and HFFT2, the particular solution approximation generated by the software was adjusted by a constant so that the approximation agreed exactly with the true solution at $(0,0)$. This adjustment was made by our software using (2.14) in Step 5 of the OSC-MD Neumann and periodic algorithms. It should be noted that the second approach described in Section 4.1 (for even N) was used in the OSC-MD periodic algorithm to solve the 1-D collocation problems.

The global errors of both the OSC-MD and SERRG2 algorithms show the approximate solutions converging, as expected, with fourth order accuracy, since doubling the number of subintervals reduces the error by a factor of 1/16. The errors in the derivative approximations converge with third order accuracy. HFFT2 solution approximations also show the expected fourth order convergence behavior. The plots of nodal errors for OSC exhibit the fourth order accuracy of the approximate solution and its first and mixed second derivative approximations. The fourth order rate of convergence in the derivative approximations at the nodes is traditionally referred to as "superconvergence".

The efficiency of the OSC-MD algorithm is demonstrated in each graph. At the nodal points of the partition, the solution accuracy obtained by OSC-MD relative to execution time is approximately an order of magnitude higher than SERRG2 with bicubic splines, while the first derivative accuracy is up to three orders of magnitude higher (see Fig. 5.2). The results are not as dramatic for the global errors for OSC-

MD, but the accuracy achieved in a given amount of execution time is still higher than SERRG2. This is not surprising, since the cost of SERRG2 is $O(N^3)$ because it involves the numerical computation of eigensystems and performs matrix-vector multiplications in a traditional way without using FFTs. HFFT2 does provide cheap, accurate solution approximations, however, it does not provide a global solution representation, nor does it provide derivative approximations. The efficiency of HFFT2 is due to the fact that, like OSC-MD, its cost is $O(N^2 \log N)$ operations, and it performs fewer FFTs than OSC-MD.

6. Concluding Remarks. Although we have emphasized in this paper the solution of singular Neumann and periodic collocation problems, the eigensystem matrices presented here and in [6] can be used to solve collocation problems with a variety of boundary condition combinations. The basic machinery of the MD algorithm does not change for these extensions; only some small details in applying the appropriate FFTs and solving the decoupled 1-D collocation problems need be altered.

The tremendous potential of the OSC-MD Algorithm in a shared or distributed memory parallel computing environment is also worthy of note. The algorithm has the advantage that each of the main computational steps (Steps 1, 2, 3 and 4), consists of 2N totally independent subtasks. In the case of Steps 1 and 4, these subtasks are matrix-vector products. In the case of Steps 2 and 3, the subtasks are independent solutions of ABD systems. In [5] and [17], the implementation of OSC-MD (for non-singular problems) on shared memory machines was addressed. The highly parallel nature of the MD algorithm becomes vital when this method is extended from two- to three-dimensional problems. In three dimensions, its memory requirements alone can preclude the solution of problems with fine partitions on serial architectures. On a distributed architecture, however, the memory requirement and computations can be spread across several processors, enabling larger problems to be solved. The implementation of OSC-MD for three-dimensional problems on distributed memory machines is addressed in [2] and [22].

REFERENCES

[1] K.R. Bennett, *Parallel collocation methods for boundary value problems*, Ph.D. thesis, University of Kentucky, Lexington, KY, 1991.

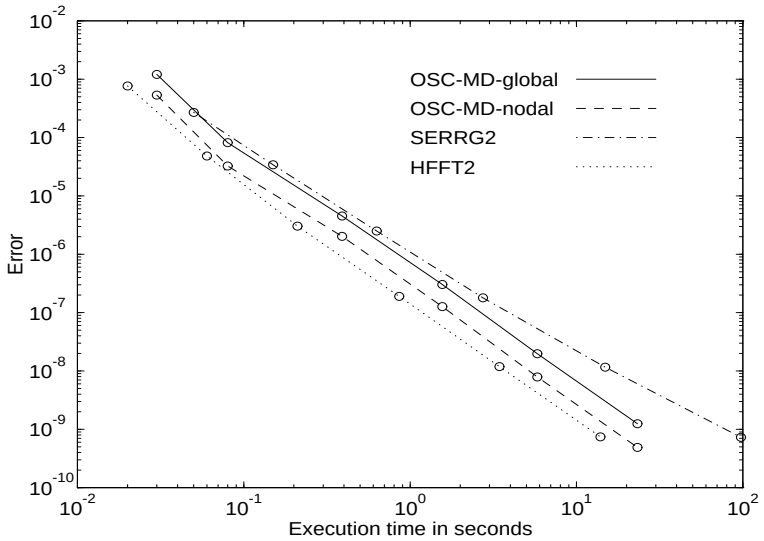

FIG. 5.1. *Results for Problem 1 showing execution time and errors in the aproximate solution for OSC-MD (global/nodal), SERRG2 and HFFT2.*

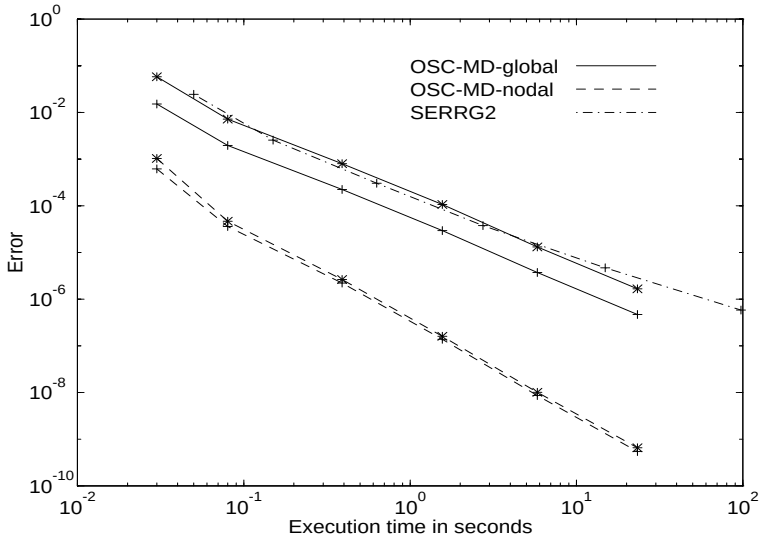

FIG. 5.2. *Results for Problem 1 showing execution time and errors in the approximate derivatives for OSC-MD (global/nodal), and SERRG2. + denotes errors in both first derivative approximations, and ∗ denotes errors in mixed second derivative approximations (OSC-MD only).*

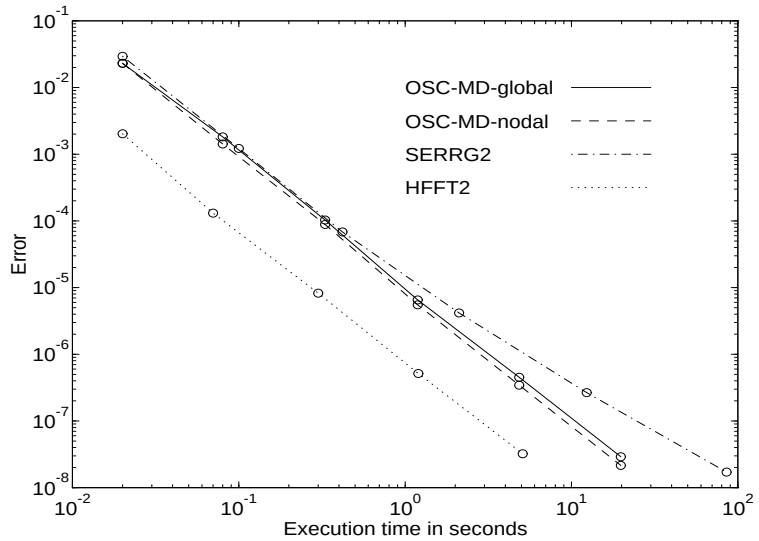

FIG. 5.3. *Results for Problem 2 showing execution time and errors in the approximate solution for OSC-MD (global/nodal), SERRG2 and HFFT2.*

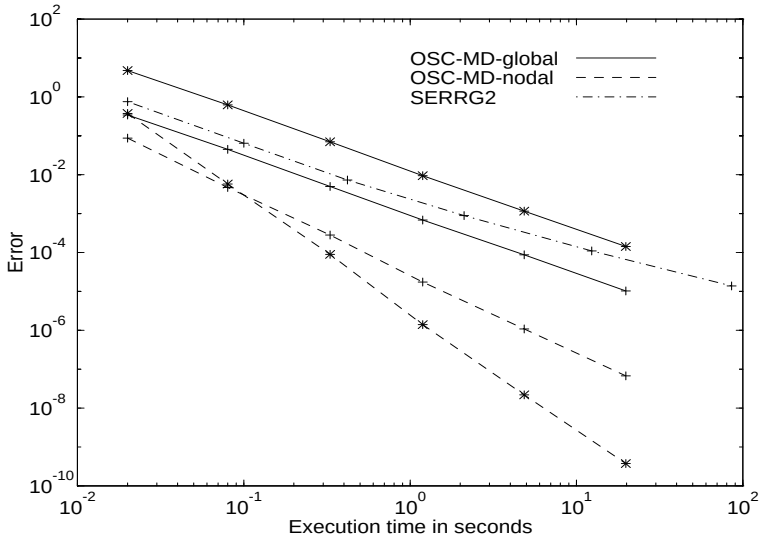

FIG. 5.4. *Results for Problem 2 showing execution time and errors in the approximate derivatives for OSC-MD (global/nodal), and SERRG2. + denotes errors in both first derivative approximations, and ∗ denotes errors in mixed second derivative approximations (OSC-MD only).*

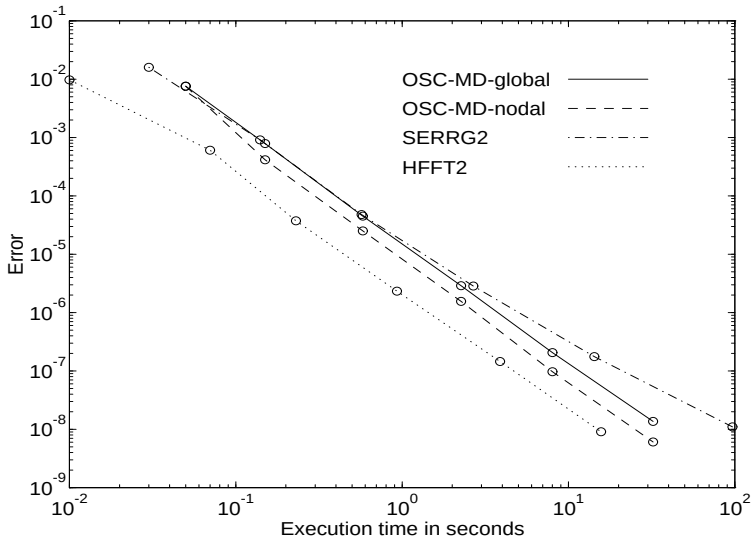

FIG. 5.5. *Results for Problem 3 showing execution time and errors in the approximate solution for OSC-MD (global/nodal), SERRG2 and HFFT2.*

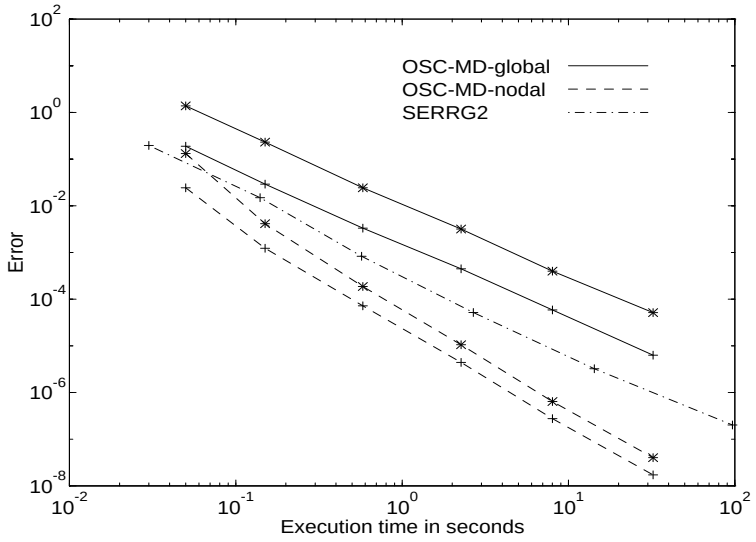

FIG. 5.6. *Results for Problem 3 showing execution time and errors in the approximate derivatives for OSC-MD (global/nodal), and SERRG2. + denotes errors in both first derivative approximations, and ∗ denotes errors in mixed second derivative approximations (OSC-MD only).*

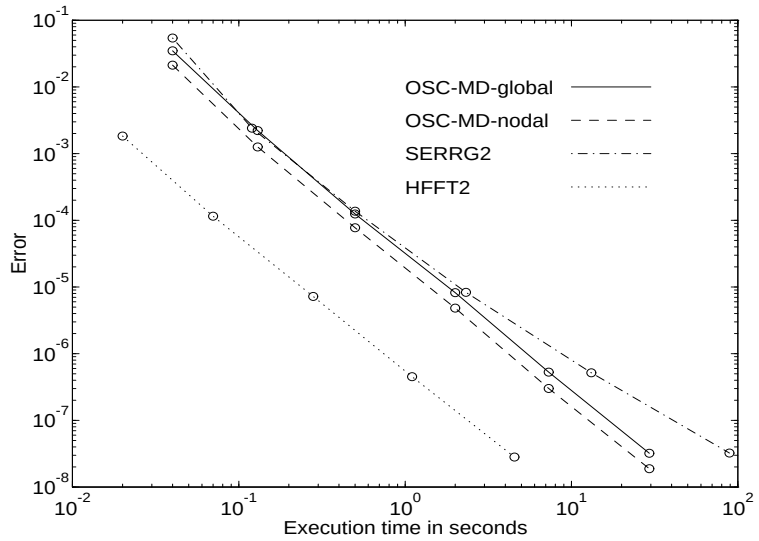

FIG. 5.7. *Results for Problem 4 showing execution time and errors in the approximate solution for OSC-MD (global/nodal), SERRG2 and HFFT2.*

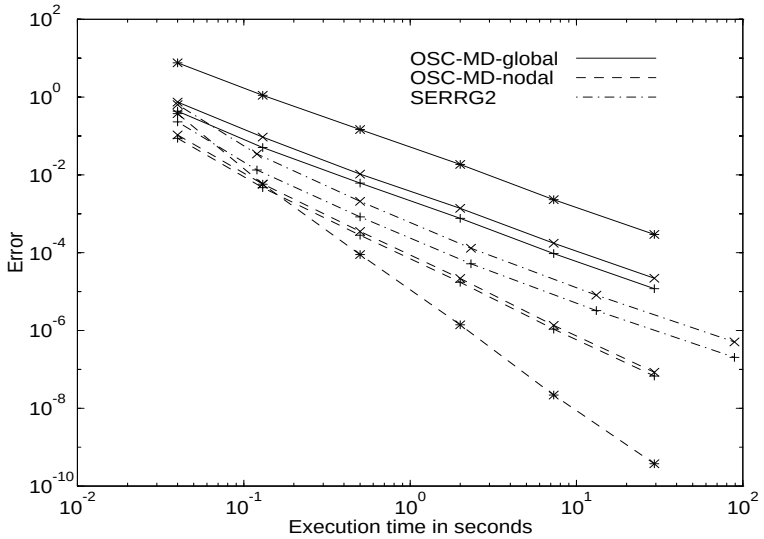

FIG. 5.8. *Results for Problem 4 showing execution time and errors in the approximate derivatives for OSC-MD (global/nodal), and SERRG2.* $+$ *and* $\times$ *denote errors in first derivative approximations with respect to* x *and* y*, respectively, and* $*$ *denotes errors in mixed second derivative approximations (OSC-MD only).*

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A. Orthogonal spline collocation eigensystem matrices. We present here the explicit formulas for the eigensystem matrices required in the Fourier transformation step of the matrix decomposition algorithms for orthogonal spline collocation. A complete derivation is given in [1], and is available on request from the first author. First we consider orthogonal spline collocation eigensystems corresponding to the Neumann boundary condition. Let $\Lambda_{\mathcal{N}}$ be the diagonal matrix given by

$$\Lambda_{\mathcal{N}} = \mathrm{diag}(\lambda_1^{\mathcal{N}}, \ldots, \lambda_{2N}^{\mathcal{N}}), \tag{A.1}$$

where

$$\lambda_{1+j}^{\mathcal{N}} = 12\left(\frac{8+\eta_j-\mu_j}{7-\eta_j}\right)h^{-2}, \qquad j = 0, \ldots, N,$$

$$\lambda_{N+1+j}^{\mathcal{N}} = 12\left(\frac{8+\eta_j+\mu_j}{7-\eta_j}\right)h^{-2}, \qquad j = 1, \ldots, N-1,$$

and

$$\eta_j = \cos\left(\frac{j\pi}{N}\right), \qquad \mu_j = \sqrt{43+40\eta_j-2\eta_j^2}.$$

It can be verified that

$$0 = \lambda_1^{\mathcal{N}} < \lambda_2^{\mathcal{N}} < \ldots < \lambda_{N+1}^{\mathcal{N}} = 9h^{-2}, \quad 36h^{-2} > \lambda_{N+2}^{\mathcal{N}} > \ldots > \lambda_{2N}^{\mathcal{N}} > 12h^{-2}. \tag{A.2}$$

Let $\Lambda_\alpha^\pm$, $\Lambda_\beta^\pm$ be diagonal matrices defined by

$$\Lambda_\alpha^- = \mathrm{diag}(\tfrac{1}{6\sqrt{3}}, \alpha_1^-, \ldots, \alpha_{N-1}^-, \tfrac{1}{8}), \qquad \Lambda_\alpha^+ = \mathrm{diag}(\alpha_1^+, \ldots, \alpha_{N-1}^+),$$

$$\Lambda_\beta^\pm = \mathrm{diag}(\beta_1^\pm, \ldots, \beta_{N-1}^\pm),$$

respectively, where

$$\alpha_j^\pm = (5 + 4\eta_j \mp \mu_j)\nu_j^\pm, \qquad \beta_j^\pm = 18 \sin\left(\frac{j\pi}{N}\right)\nu_j^\pm,$$

and

$$\nu_j^\pm = \left[27(1+\eta_j)(8+\eta_j \mp \mu_j)^2 + (1-\eta_j)(11+7\eta_j \mp 4\mu_j)^2\right]^{-1/2}.$$

Finally, let $Z_{\mathcal{N}}$ be defined by

$$\text{(A.3)} \qquad Z_{\mathcal{N}} = (z_{m,n}^{\mathcal{N}})_{m,n=1}^{2N} = 3\left(\frac{6}{N}\right)^{1/2} \left[\begin{array}{c|c|c|c} C\Lambda_\alpha^- & & & \tilde{C}\Lambda_\alpha^+ \\ \hline \mathbf{0} & -S\Lambda_\beta^- & \mathbf{0} & -S\Lambda_\beta^+ \end{array}\right],$$

where $\mathbf{0}$ is the $(N-1)$-dimensional zero column vector, and the matrices S, C, $\tilde{C}$ are given respectively by

$$S = \left(\sin\frac{mn\pi}{N}\right)_{m,n=1}^{N-1}, \qquad C = \left(\cos\frac{mn\pi}{N}\right)_{m,n=0}^{N},$$

$$\tilde{C} = \left(\cos\frac{mn\pi}{N}\right)_{m=0,n=1}^{N,N-1}.$$

If the matrices A_x and B_x are defined by (3.8) with $\{\phi_n\}_{n=1}^{2N}$ of (3.2), then, see Theorem 8.3 in [1] (cf. Theorem 2.2 in [5]),

$$\text{(A.4)} \qquad Z_{\mathcal{N}}^T B_x^T A_x Z_{\mathcal{N}} = \Lambda_{\mathcal{N}}, \qquad Z_{\mathcal{N}}^T B_x^T B_x Z_{\mathcal{N}} = I,$$

where I is the identity matrix of order $2N$.

We now consider orthogonal spline collocation matrices associated with the periodic boundary conditions, taking N to be an even integer. (For the corresponding results for odd values of N, see [1].) Let $\Lambda_{\mathcal{P}}$ be diagonal matrix given by

$$\text{(A.5)} \qquad \Lambda_{\mathcal{P}} = \mathrm{diag}(\lambda_1^{\mathcal{P}}, \ldots, \lambda_{2N}^{\mathcal{P}}),$$

where

$$\lambda_{1+j}^{\mathcal{P}} = \lambda_{1+2j}^{\mathcal{N}}, \qquad \lambda_{N+2+j}^{\mathcal{P}} = \lambda_{N+1+2j}^{\mathcal{N}}, \qquad j = 0, \ldots, N/2-1,$$

$$\lambda^p_{N/2+1} = 12h^{-2}, \qquad \lambda^p_{N/2+2} = 36h^{-2},$$

$$\lambda^p_{N/2+1+j} = \lambda^p_j\,, \qquad \lambda^p_{3N/2+j} = \lambda^p_{N+1+j}\,, \qquad j = 2, \ldots, N/2.$$

Let $\Lambda^{\pm}_{\alpha}$, $\Lambda^{\pm}_{\beta}$ be diagonal matrices defined now by

$$\Lambda^-_\alpha = \mathrm{diag}(\tfrac{1}{6\sqrt{3}}, \hat\alpha^-_1, \ldots, \hat\alpha^-_{N/2-1}, \tfrac{1}{8}), \qquad \Lambda^+_\alpha = \mathrm{diag}(\hat\alpha^+_1, \ldots, \hat\alpha^+_{N/2-1}),$$

$$\Lambda^-_\beta = \mathrm{diag}(1, \hat\beta^-_1, \ldots, \hat\beta^-_{N/2-1}, \tfrac{1}{\sqrt{3}}), \qquad \Lambda^+_\beta = \mathrm{diag}(\hat\beta^+_1, \ldots, \hat\beta^+_{N/2-1}),$$

where $\hat\alpha^{\pm}_j = \alpha^{\pm}_{2j}$ and $\hat\beta^{\pm}_j = \beta^{\pm}_{2j}$. Let Z_p be defined by

$$\text{(A.6)} \qquad Z_p = (z^p_{m,n})^{2N}_{m,n=1} = 3\left(\frac{6}{N}\right)^{1/2} \left[\begin{array}{c|c|c|c} -\tilde C\Lambda^-_\alpha & \tilde S\Lambda^-_\alpha & -C\Lambda^+_\alpha & S\Lambda^+_\alpha \\ \hline \tilde S\Lambda^-_\beta & \tilde C\Lambda^-_\beta & S\Lambda^+_\beta & C\Lambda^+_\beta \end{array}\right].$$

where the matrices $S, C, \tilde S$ and $\tilde C$ are given now by

$$S = \left(\sin\frac{(2m-1)n\pi}{N}\right)^{N,N/2-1}_{m,n=1}, \qquad C = \left(\cos\frac{(2m-1)n\pi}{N}\right)^{N,N/2-1}_{m,n=1},$$

$$\tilde C = \left(\cos\frac{(2m-1)n\pi}{N}\right)^{N,N/2}_{m=1,n=0}, \qquad \tilde S = \left(\sin\frac{(2m-1)n\pi}{N}\right)^{N,N/2}_{m=1,n=0}.$$

If the matrices A_x and B_x are defined by (3.8) with $\{\phi_n\}^{2N}_{n=1}$ of (4.1), then, see Theorem 8.6 in [1],

$$\text{(A.7)} \qquad Z^T_p B^T_x A_x Z_p = \Lambda_p\,, \qquad Z^T_p B^T_x B_x Z_p = I.$$