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Direct and iterative solution of the generalized Dirichlet–Neumann map for elliptic PDEs on square domains[☆]

A.G. Sifalakis [a], S.R. Fulton [b], E.P. Papadopoulou [a], Y.G. Saridakis [a,*]

[a] *Applied Mathematics and Computers Lab, Department of Sciences, Technical University of Crete, 73100 Chania, Greece*

[b] *Department of Mathematics and Computer Science, Clarkson University, Potsdam NY 13699-5815, USA*

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ABSTRACT

In this work we derive the structural properties of the Collocation coefficient matrix associated with the Dirichlet–Neumann map for Laplace's equation on a square domain. The analysis is independent of the choice of basis functions and includes the case involving the same type of boundary conditions on all sides, as well as the case where different boundary conditions are used on each side of the square domain. Taking advantage of said properties, we present efficient implementations of direct factorization and iterative methods, including classical SOR-type and Krylov subspace (Bi-CGSTAB and GMRES) methods appropriately preconditioned, for both Sine and Chebyshev basis functions. Numerical experimentation, to verify our results, is also included.

1. Introduction

Recently, Fokas [1,4] introduced a new unified approach for analyzing linear and integrable nonlinear PDEs. A central issue to this approach is a generalized Dirichlet to Neumann map, characterized through the solution of the so-called *global relation*, namely, an equation, valid for all values of an *arbitrary* complex parameter k, coupling specified known and unknown values of the solution and its derivatives on the boundary. In particular, for the case of the complex form of *Laplace's equation*

$$
\begin{aligned}
&q_{z\bar{z}} \equiv \frac{\partial^2 q}{\partial z \partial \bar{z}} = 0 \Leftrightarrow \frac{\partial}{\partial \bar{z}}\left(\mathrm{e}^{-\mathrm{i}kz}\frac{\partial q}{\partial z}\right) = 0, \quad k \in \mathbb{C} \text{ is arbitrary},\\
&(z,\bar{z}) = (x+\mathrm{i}y, x-\mathrm{i}y), \qquad q_z = \frac{1}{2}\left(q_x - \mathrm{i}q_y\right), \qquad q_{\bar{z}} = \frac{1}{2}\left(q_x + \mathrm{i}q_y\right), \quad \mathrm{i}^2 = -1,
\end{aligned}
$$

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* Corresponding author.
E-mail address: yiannis@science.tuc.gr (Y.G. Saridakis).

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in a convex bounded polygon D with vertices $z_1, z_2, \ldots, z_n$(modulo n) indexed counterclockwise, the associated *Global Relation* takes the form (see also [2,3])

$$\sum_{j=1}^{n} \varrho_j(k) = 0, \qquad \varrho_j(k) \doteq \int_{S_j} \mathrm{e}^{-\mathrm{i}kz} q_z \mathrm{d}z, \quad k \in \mathbb{C}, \tag{1.1}$$

where $k \in \mathbb{C}$ is arbitrary and S_j denotes the side from z_j to z_{j+1} (not including the end points). At this point we remark that, as Fokas has shown in [4], there also holds

$$q_z = \frac{1}{2\pi} \sum_{j=1}^{n} \int_{\ell_j} \mathrm{e}^{\mathrm{i}kz} \varrho_j(k) \mathrm{d}k, \quad \ell_j \doteq \left\{k \in \mathbb{C} : \arg(k) = -\arg(z_j - z_{j+1})\right\},$$

hence

$$q = 2\mathrm{Re} \int_{z_0}^{z} q_z \mathrm{d}z + \text{const.}$$

It is therefore apparent that the *spectral functions* $\varrho_j(k)$ in (1.1) play a crucial role in the solution of Laplace's equation. To determine them, for $z \in S_j$, $1 \le j \le n$, we first let

- $q_\tau^{(j)}$ denote the *tangential* component of q_z along the side S_j,
- $q_n^{(j)}$ denote the outward *normal* component of q_z along the side S_j,
- $g^{(j)}$ denote the derivative of the solution in the direction making an angle β_j, $0 \le \beta_j \le \pi$, with the side S_j, namely:

$$\cos\left(\beta_j\right) q_\tau^{(j)} + \sin\left(\beta_j\right) q_n^{(j)} = g^{(j)}, \tag{1.2}$$

- $f^{(j)}$ denote the derivative of the solution in the direction normal to the above direction, namely:

$$-\sin\left(\beta_j\right) q_\tau^{(j)} + \cos\left(\beta_j\right) q_n^{(j)} = f^{(j)}. \tag{1.3}$$

Then, by using the identity

$$\frac{\partial q}{\partial z} = \frac{1}{2} \mathrm{e}^{-\mathrm{i}\alpha_j} \left(q_\tau^{(j)} + \mathrm{i} q_n^{(j)}\right), \quad z \in S_j, \qquad \alpha_j = \arg\left(z_{j+1} - z_j\right), \tag{1.4}$$

and substituting into the *Global Relation* (1.1) we obtain (cf. [2,3]) the *Generalized Dirichlet–Neumann map*, that is the relation between the sets $\left\{f^{(j)}(s)\right\}$ and $\left\{g^{(j)}(s)\right\}_{j=1}^{n}$, which is characterized by the single equation

$$\sum_{j=1}^{n} \left|h_j\right| \mathrm{e}^{\mathrm{i}\left(\beta_j - km_j\right)} \int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}kh_j s} \left(f^{(j)} - \mathrm{i}g^{(j)}\right) \mathrm{d}s = 0, \quad k \in \mathbb{C} \tag{1.5}$$

where, $k \in \mathbb{C}$ is arbitrary and for $j = 1, 2, \ldots, n$, and $z_{n+1} = z_1$,

$$h_j := \frac{1}{2\pi}\left(z_{j+1} - z_j\right), \qquad m_j := \frac{1}{2}\left(z_{j+1} + z_j\right), \qquad s := \frac{z - m_j}{h_j}. \tag{1.6}$$

For the numerical solution of the Generalized Dirichlet–Neumann map in (1.5), a Collocation-type method has been developed (see [2,3]): Suppose that the set $\left\{g^{(j)}(s)\right\}_{j=1}^{n}$ is given through the boundary conditions, and that $\left\{f^{(j)}(s)\right\}_{j=1}^{n}$ is approximated by $\left\{f_N^{(j)}(s)\right\}_{j=1}^{n}$ where

$$f_N^{(j)}(s) = f_*^{(j)}(s) + \sum_{r=1}^{N} U_r^j \varphi_r(s), \tag{1.7}$$

with N being an even integer, $2\pi f_*^{(j)}(s) := (s+\pi) f^{(j)}(\pi) - (s-\pi) f^{(j)}(-\pi)$ (the values of $f^{(j)}(\pi)$ and $f^{(j)}(-\pi)$ can be computed by the continuity requirements at the vertices of the polygon), and the set of real-valued linearly independent functions $\{\varphi_r(s)\}_{r=1}^{N}$ being the *basis* functions. If we evaluate Eq. (1.5) on the following n-rays of the complex k-plane: $k_p = -\frac{l}{h_p}$, $l \in \mathbb{R}^+$, $p = 1, \ldots, n$, then the real coefficients U_r^j satisfy the system of linear algebraic equations

$$\sum_{j=1}^{n} \frac{\left|h_j\right|}{\left|h_p\right|} \mathrm{e}^{\mathrm{i}\left(\beta_j - \beta_p\right)} \mathrm{e}^{-\mathrm{i}\frac{l}{h_p}\left(m_p - m_j\right)} \sum_{r=1}^{N} U_r^j \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}l\frac{h_j}{h_p}s} \varphi_r(s) \mathrm{d}s = G_p(l) \tag{1.8}$$

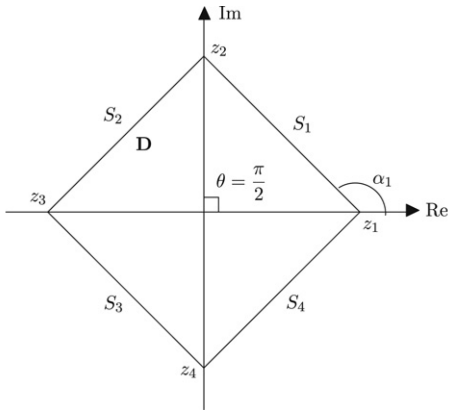

Fig. 2.1. Square domain with vertices z_j, sides S_j and interior **D**.

where $G_p(l)$ denotes the known function

$$G_p\,(l) = \mathrm{i}\sum_{j=1}^{n} \frac{|h_j|}{|h_p|} \mathrm{e}^{\mathrm{i}(\beta_j-\beta_p)} \mathrm{e}^{-\mathrm{i}\frac{l}{h_p}(m_p-m_j)} \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}l\frac{h_j}{h_p}s} \left(g^{(j)}\,(s) + \mathrm{i}f_*^{(j)}\,(s)\right) \mathrm{d}s, \tag{1.9}$$

and l is chosen as follows: $l = \frac{1}{2}, \frac{3}{2}, \ldots, \frac{N-1}{2}$ and $l = 1, 2, \ldots, \frac{N}{2}$ for the real and imaginary parts of Eq. (1.8), respectively, defining a set of *Collocation points*.

2. Collocation matrix structure for square domains

Consider, now, the square with vertices z_j and sides S_j, $j = 1, 2, 3, 4$ (modulo 4), indexed counterclockwise, and interior **D**, depicted in Fig. 2.1. Without any loss of generality, we may assume that the square is centered at the origin, scaled and oriented so that one vertex (say z_1) is located at 1, hence

$$z_j = \mathrm{i}^{j-1}, \quad j = 1, 2, 3, 4 \tag{2.1}$$

and the angle α_j of the side S_j from the real axis (measured counterclockwise) is given by

$$\alpha_j = \arg(z_{j+1} - z_j) = (2j+1)\frac{\pi}{4}, \quad j = 1, 2, 3, 4. \tag{2.2}$$

Case I: Same boundary conditions on all sides

Assuming that the real-valued function $q\,(z, \bar{z})$ satisfies Laplace's equation in the interior **D** of the square, described above, subject to the same type of Poincaré boundary conditions on all sides, that is

$$\cos\,(\beta)\,q_s^{(j)} + \sin\,(\beta)\,q_n^{(j)} = g^{(j)}, \quad z \in S_j,\ 1 \le j \le 4, \tag{2.3}$$

and observing that the local coordinates of (1.6) take the forms

$$m_j = \frac{1}{2}\left(z_j + z_{j+1}\right) = |m_j|\mathrm{e}^{\mathrm{i}(\alpha_j - \frac{\pi}{2})} = \frac{1}{\sqrt{2}}\mathrm{e}^{\mathrm{i}(2j-1)\frac{\pi}{4}} = \frac{1}{\sqrt{2}}\mathrm{i}^{(2j-1)/2}, \tag{2.4}$$

and

$$h_j = \frac{1}{2\pi}\left(z_{j+1} - z_j\right) = |h_j|\mathrm{e}^{\mathrm{i}\alpha_j} = \frac{1}{\pi\sqrt{2}}\mathrm{e}^{\mathrm{i}(2j+1)\frac{\pi}{4}} = \frac{1}{\pi\sqrt{2}}\mathrm{i}^{(2j+1)/2}, \tag{2.5}$$

we can easily obtain, from (1.5), that:

Lemma 2.1. *Let the real-valued function $q\,(z, \bar{z})$ satisfy Laplace's equation in the interior D of the square described above in this section. Let $g^{(j)}$ denote the derivative of the solution in the direction making an angle β, $0 \le \beta \le \pi$, with the side S_j (see (2.3)), and let $f^{(j)}$ denote the derivative of the solution in the direction normal to the above direction. The generalized Dirichlet–Neumann map is characterized by the equation*

$$\sum_{j=1}^{4} \mathrm{e}^{-kM_j} \int_{-\pi}^{\pi} \mathrm{e}^{-kH_j s} \left(f^{(j)}(s) - \mathrm{i}g^{(j)}(s)\right) \mathrm{d}s = 0, \quad k \in \mathbb{C}, \tag{2.6}$$

where

$$M_j = \mathrm{i}m_j = \frac{1}{\sqrt{2}}\mathrm{i}^{(2j+1)/2} \quad \textit{and} \quad H_j = \mathrm{i}h_j = \frac{1}{\pi\sqrt{2}}\mathrm{i}^{(2j+3)/2}. \tag{2.7}$$

Proof. Upon simplification of the factors $|h_j|$ and $\mathrm{e}^{\mathrm{i}\beta_j}$, as $|h_j| = \frac{1}{2\pi}$ and $\beta_j = \beta$, from (1.5), the proof follows immediately. □

Hence, upon evaluation of (2.6) on the following four rays of the complex k-plane

$$k_p = -\frac{l}{h_p}, \quad l \in \mathbb{R}^+, p = 1, 2, 3, 4, \tag{2.8}$$

we obtain that:

Proposition 2.1. *Consider the generalized Dirichlet–Neumann map in Lemma 2.1. Suppose that the set* $\left\{g^{(j)}\right\}_{j=1}^4$ *is given through (2.3) and that the set* $\left\{f^{(j)}\right\}_{j=1}^4$ *is approximated by* $\left\{f_N^{(j)}\right\}_{j=1}^4$ *defined in (1.7). Then, the real coefficients* U_r^j *satisfy the* $4N \times 4N$ *linear system of equations*

$$\sum_{j=1}^{4} \mathrm{e}^{l\pi \mathrm{i}^{j-p}} \sum_{r=1}^{N} U_r^j F_r\left(l\mathrm{i}^{j-p}\right) = G_p\left(l\right), \quad p = 1, 2, 3, 4, \tag{2.9}$$

where $G_p\left(l\right)$ *denotes the known function*

$$G_p\left(l\right) = \mathrm{i}\sum_{j=1}^{4} \mathrm{e}^{l\pi \mathrm{i}^{j-p}} \int_{-\pi}^{\pi} \mathrm{e}^{ls\mathrm{i}^{j-p+1}} (g^{(j)}(s) + \mathrm{i}f_*^{(j)}(s))\mathrm{d}s, \tag{2.10}$$

$F_r\left(l\right)$ *denotes the integral*

$$F_r\left(l\right) = \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}ls}\varphi_r(s)\mathrm{d}s, \quad r = 1, 2, \ldots, N, \tag{2.11}$$

and l *is chosen as follows: For the real part of Eq. (2.9)* $l = \frac{1}{2}, \frac{3}{2}, \ldots, \frac{N-1}{2}$, *whereas for the imaginary part of Eq. (2.9)* $l = 1, 2, \ldots, N/2$.

Proof. Observe that

$$\frac{M_j}{h_p} = \pi\mathrm{i}^{j-p} \quad \text{and} \quad \frac{H_j}{h_p} = \mathrm{i}^{j-p+1}. \tag{2.12}$$

Thus, evaluation of (2.6) at (2.8) yields the set of the four equations

$$\sum_{j=1}^{4} \mathrm{e}^{l\pi \mathrm{i}^{j-p}} \int_{-\pi}^{\pi} \mathrm{e}^{ls\mathrm{i}^{j-p+1}} \left(f^{(j)}(s) - \mathrm{i}g^{(j)}(s)\right)\mathrm{d}s = 0, \quad l \in \mathbb{R}^+, p = 1, 2, 3, 4, \tag{2.13}$$

hence, the proof follows immediately upon substitution of (1.7) into (2.13). □

If we now let $A_{p,j} \in \mathbb{R}^{N,N}(p, j = 1, 2, 3, 4)$, denote the $N \times N$ matrix with elements $a_{q,r}^{p,j}$ defined by

$$a_{q,r}^{p,j} = \begin{cases} \mathrm{Re}\left(\mathrm{e}^{l\pi \mathrm{i}^{j-p}} \int_{-\pi}^{\pi} \mathrm{e}^{ls\mathrm{i}^{j-p+1}}\varphi_r(s)\mathrm{d}s\right), & l = \frac{1}{2}, \frac{3}{2}, \ldots, \frac{N-1}{2} \\ \mathrm{Im}\left(\mathrm{e}^{l\pi \mathrm{i}^{j-p}} \int_{-\pi}^{\pi} \mathrm{e}^{ls\mathrm{i}^{j-p+1}}\varphi_r(s)\mathrm{d}s\right), & l = 1, 2, \ldots, N/2, \end{cases} \tag{2.14}$$

for $q = 2l$ and $r = 1, 2, \ldots, N$, then the Collocation linear system, described in Proposition 2.1, may be written as

$$A_C\mathbf{U} = \mathbf{G}, \quad A_C \in \mathbb{R}^{4N,4N}, \mathbf{U}, \mathbf{G} \in \mathbb{R}^{4N}, \tag{2.15}$$

where

$$A_C = \begin{pmatrix} A_{1,1} & A_{1,2} & A_{1,3} & A_{1,4} \\ A_{2,1} & A_{2,2} & A_{2,3} & A_{2,4} \\ A_{3,1} & A_{3,2} & A_{3,3} & A_{3,4} \\ A_{4,1} & A_{4,2} & A_{4,3} & A_{4,4} \end{pmatrix}, \quad \mathbf{U} = \begin{pmatrix} \mathbf{U}_1 \\ \mathbf{U}_2 \\ \mathbf{U}_3 \\ \mathbf{U}_4 \end{pmatrix}, \quad \mathbf{G} = \begin{pmatrix} \mathbf{G}_1 \\ \mathbf{G}_2 \\ \mathbf{G}_3 \\ \mathbf{G}_4 \end{pmatrix} \tag{2.16}$$

and $\mathbf{U}_j \in \mathbb{R}^{N,1}$ and $\mathbf{G}_p \in \mathbb{R}^{N,1}$ denote the real vectors

$$\mathbf{U}_j = \left\{U_r^j\right\}_{r=1}^{N} = \begin{pmatrix} U_1^j & U_2^j & \dots & U_N^j \end{pmatrix}^{\mathrm{T}}, \tag{2.17}$$

and

$$\mathbf{G}_p = \left\{G_q^p\right\}_{q=1}^{N} = \begin{pmatrix} G_1^p & G_2^p & \dots & G_N^p \end{pmatrix}^{\mathrm{T}}, \tag{2.18}$$

with

$$G_q^p = \begin{cases} \mathrm{Re}\left(G_p(l)\right), & l = \dfrac{1}{2}, \dfrac{3}{2}, \dots, \dfrac{N-1}{2}, \\ \mathrm{Im}\left(G_p(l)\right), & l = 1, 2, \dots, N/2, \end{cases} \qquad q = 2l. \tag{2.19}$$

Following the notation above we prove:

Lemma 2.2. *The $N \times N$ real submatrices $A_{p,j} = \left\{a_{q,r}^{p,j}\right\}$, with $a_{q,r}^{p,j}$ being as defined in (2.14), satisfy*

$$A_{p,j} = E \begin{cases} A_0, & p = j \\ A_1, & |p-j| = 2 \\ O, & |p-j| = 1, 3, \end{cases} \tag{2.20}$$

where the elements of the matrix $A_0 = \left\{a_{q,r}\right\}_{q,r=1}^{N}$ are defined through the Finite Cosine/Sine Fourier Transform of the linear independent real-valued basis functions $\phi_r(s)$, namely

$$a_{q,r} = \begin{cases} \displaystyle\int_{-\pi}^{\pi} \cos\left(\frac{q}{2}s\right)\phi_r(s)\mathrm{d}s, & q = odd \\ \displaystyle\int_{-\pi}^{\pi} \sin\left(\frac{q}{2}s\right)\phi_r(s)\mathrm{d}s, & q = even, \end{cases} \tag{2.21}$$

the matrix A_1 is defined by

$$A_1 = DA_0, \qquad D = \mathrm{diag}(d_1, \dots, d_N), \qquad d_q = (-1)^{q-1}\mathrm{e}^{-q\pi}, \quad q = 1, \dots, N, \tag{2.22}$$

the matrix O denotes the null matrix and the diagonal matrix E is defined by

$$E = \mathrm{diag}(e_1, \dots, e_N), \qquad e_q = \mathrm{e}^{\frac{q}{2}\pi}, \quad q = 1, \dots, N. \tag{2.23}$$

Proof. Recall the definition of the elements $a_{q,r}^{p,j}$ from (2.14) and notice that, for $j = p$, there holds

$$a_{q,r}^{p,p} = \mathrm{e}^{l\pi} \begin{cases} \mathrm{Re}\left(\displaystyle\int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}ls}\varphi_r(s)\mathrm{d}s\right), & l = \dfrac{1}{2}, \dfrac{3}{2}, \dots, \dfrac{N-1}{2} \\ \mathrm{Im}\left(\displaystyle\int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}ls}\varphi_r(s)\mathrm{d}s\right), & l = 1, 2, \dots, N/2 \end{cases} \qquad q = 2l.$$

Evidently, therefore,

$$a_{q,r}^{p,p} = \mathrm{e}^{\frac{q}{2}\pi} a_{q,r} \tag{2.24}$$

where $a_{q,r}$ are as defined in (2.21), hence

$$A_{p,p} = EA_0, \quad p = 1, 2, 3, 4. \tag{2.25}$$

Similarly, as $\mathrm{i}^{j-p} = -1$ for $|j-p| = 2$, there holds

$$a_{q,r}^{p,j} = \mathrm{e}^{-l\pi} \begin{cases} \mathrm{Re}\left(\displaystyle\int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}ls}\varphi_r(s)\mathrm{d}s\right) = \displaystyle\int_{-\pi}^{\pi} \cos(ls)\phi_r(s)\mathrm{d}s, & l = \dfrac{1}{2}, \dfrac{3}{2}, \dots, \dfrac{N-1}{2} \\ \mathrm{Im}\left(\displaystyle\int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}ls}\varphi_r(s)\mathrm{d}s\right) = -\displaystyle\int_{-\pi}^{\pi} \sin(ls)\phi_r(s)\mathrm{d}s, & l = 1, 2, \dots, N/2, \end{cases}$$

with $q = 2l$. Hence, for $|j-p| = 2$,

$$a_{q,r}^{p,j} = (-1)^{q-1}\mathrm{e}^{-\frac{q}{2}\pi} a_{q,r} = \mathrm{e}^{\frac{q}{2}\pi}\left((-1)^{q-1}\mathrm{e}^{-q\pi} a_{q,r}\right), \tag{2.26}$$

and therefore

$$A_{p,j} = EDA_0 = EA_1, \qquad |p-j| = 2. \tag{2.27}$$

Finally, for $|j-p| = \text{odd}$, we have

$$a_{q,r}^{p,j} = \left(\int_{-\pi}^{\pi} \mathrm{e}^{\pm ls}\varphi_r(s)\mathrm{d}s\right)\begin{cases}\mathrm{Re}\left(\mathrm{e}^{\pm \mathrm{i}l\pi}\right) = \cos(l\pi) = 0, & l = \frac{1}{2}, \frac{3}{2}, \ldots, \frac{N-1}{2}\\ \mathrm{Im}\left(\mathrm{e}^{\pm \mathrm{i}l\pi}\right) = \pm\sin(l\pi) = 0, & l = 1, 2, \ldots, N/2,\end{cases}$$

and, therefore,

$$A_{p,j} = O, \qquad |p-j| = \text{odd}, \tag{2.28}$$

which completes the proof. □

Therefore, it becomes apparent that:

Proposition 2.2. *The Collocation linear system in (2.15) is equivalent to the system*

$$A\mathbf{U} = (I_4 \otimes E^{-1})\mathbf{G}, \tag{2.29}$$

where ⊗ denotes the Kronecker (tensor) matrix product, A is defined by

$$A = \begin{pmatrix} A_0 & O & A_1 & O \\ O & A_0 & O & A_1 \\ A_1 & O & A_0 & O \\ O & A_1 & O & A_0 \end{pmatrix} = \begin{pmatrix} I & O & D & O \\ O & I & O & D \\ D & O & I & O \\ O & D & O & I \end{pmatrix}(I_4 \otimes A_0), \tag{2.30}$$

I_4 denotes the 4×4 identity matrix, and the matrices A_0, A_1, D and E are as defined in Lemma 2.2.

Remark 2.1. Notice that, as the basis functions $\varphi_r(s)$ are appropriately chosen real-valued linearly independent functions, A_0 is nonsingular. The matrix B, defined by

$$B = \begin{pmatrix} I & O & D & O \\ O & I & O & D \\ D & O & I & O \\ O & D & O & I \end{pmatrix}, \tag{2.31}$$

is also nonsingular as it is apparently symmetric, strictly diagonally dominant and positive definite. Therefore, both matrices A in (2.30) and A_C in (2.16) are nonsingular too.

Remark 2.2. Observe that the matrix A in (2.30) is evidently *Block Circulant*. Naturally therefore, as $A_C = (I_4 \otimes E)A$, the Collocation matrix A_C in (2.16) is *Block Circulant* too. It was shown in [5] that although the Collocation coefficient matrix does not possess the special sparse structure of (2.30), it remains *Block Circulant* for the case of general *Regular Polygons* with the same type of boundary conditions on all sides, allowing the deployment of FFT for the efficient solution of the corresponding Collocation linear system.

Case II: Different boundary conditions on each side

Let us now assume that the real-valued function $q(z, \bar{z})$ satisfies Laplace's equation in the interior **D** of the square, described at the beginning of this section, subject to different type of *oblique Neumann* boundary conditions on each side, that is (see also Eq. (1.2))

$$\cos\left(\beta_j\right) q_s^{(j)} + \sin\left(\beta_j\right) q_n^{(j)} = g^{(j)}, \quad z \in S_j, 1 \le j \le 4. \tag{2.32}$$

Then, the associated generalized Dirichlet–Neumann map is characterized by the equation

$$\sum_{j=1}^{4} \mathrm{e}^{\mathrm{i}\beta_j}\mathrm{e}^{-kM_j}\int_{-\pi}^{\pi}\mathrm{e}^{-kH_j s}\left(f^{(j)}(s) - \mathrm{i}g^{(j)}(s)\right)\mathrm{d}s = 0, \quad k \in \mathbb{C}, \tag{2.33}$$

where M_j and H_j are as defined in Lemma 2.1, while Proposition 2.1 is being replaced by:

Proposition 2.3. *Consider the generalized Dirichlet–Neumann map in (2.33). Suppose that the set $\left\{g^{(j)}\right\}_{j=1}^4$ is given through (2.32) and that the set $\left\{f^{(j)}\right\}_{j=1}^4$ is approximated by $\left\{f_N^{(j)}\right\}_{j=1}^4$ defined in (1.7). Then, the real coefficients U_r^j satisfy the $4N \times 4N$ linear system of equations*

$$\sum_{j=1}^{4} \mathrm{e}^{\mathrm{i}\beta_j}\mathrm{e}^{l\pi\mathrm{i}^{j-p}}\sum_{r=1}^{N} U_r^j F_r\left(l\mathrm{i}^{j-p}\right) = G_p(l), \quad p = 1, 2, 3, 4, \tag{2.34}$$

where $G_p(l)$ denotes the known function

$$G_p(l) = \mathrm{i}\sum_{j=1}^{4} \mathrm{e}^{\mathrm{i}\beta_j}\mathrm{e}^{l\pi \mathrm{i}^{j-p}} \int_{-\pi}^{\pi} \mathrm{e}^{ls\mathrm{i}^{j-p+1}} (g^{(j)}(s) + \mathrm{i}f_*^{(j)}(s))\mathrm{d}s, \tag{2.35}$$

$F_r(l)$ is as in (2.11) and l is chosen as in Proposition 2.1.

The Collocation linear system, described in Proposition 2.3, obviously is in the block partitioned form of (2.16) with the difference that the elements $\alpha_{q,r}^{p,j}$ of the submatrices $A_{p,j}$, used to define the Collocation matrix A_C in (2.16), are now defined by

$$\alpha_{q,r}^{p,j} = \begin{cases} \mathrm{Re}\left(\mathrm{e}^{\mathrm{i}\beta_j}\mathrm{e}^{l\pi \mathrm{i}^{j-p}} \displaystyle\int_{-\pi}^{\pi} \mathrm{e}^{ls\mathrm{i}^{j-p+1}} \varphi_r(s)\mathrm{d}s\right), & l = \dfrac{1}{2}, \dfrac{3}{2}, \ldots, \dfrac{N-1}{2} \\ \mathrm{Im}\left(\mathrm{e}^{\mathrm{i}\beta_j}\mathrm{e}^{l\pi \mathrm{i}^{j-p}} \displaystyle\int_{-\pi}^{\pi} \mathrm{e}^{ls\mathrm{i}^{j-p+1}} \varphi_r(s)\mathrm{d}s\right), & l = 1, 2, \ldots, N/2, \end{cases} \tag{2.36}$$

and, of course, the vector $\mathbf{G}$ now refers to (2.35) instead of (2.10). It takes only a few simple algebraic manipulations to verify that

$$\alpha_{q,r}^{p,j} = a_{q,r}^{p,j}\cos(\beta_j) + \hat{a}_{q,r}^{p,j}\sin(\beta_j), \tag{2.37}$$

where $a_{q,r}^{p,j}$ is as defined in (2.14) and $\hat{a}_{q,r}^{p,j}$ is defined by

$$\hat{a}_{q,r}^{p,j} = \begin{cases} -\mathrm{Im}\left(\mathrm{e}^{l\pi \mathrm{i}^{j-p}} \displaystyle\int_{-\pi}^{\pi} \mathrm{e}^{ls\mathrm{i}^{j-p+1}} \varphi_r(s)\mathrm{d}s\right), & l = \dfrac{1}{2}, \dfrac{3}{2}, \ldots, \dfrac{N-1}{2} \\ \mathrm{Re}\left(\mathrm{e}^{l\pi \mathrm{i}^{j-p}} \displaystyle\int_{-\pi}^{\pi} \mathrm{e}^{ls\mathrm{i}^{j-p+1}} \varphi_r(s)\mathrm{d}s\right), & l = 1, 2, \ldots, N/2, \end{cases} \tag{2.38}$$

with $q = 2l$ as always. Therefore,using also Proposition 2.2, the Collocation coefficient matrix A_C now takes the form

$$A_C = (I_4 \otimes E)\,A\,(D_c \otimes I_N) + \hat{A}\,(D_s \otimes I_N), \tag{2.39}$$

where the matrices A and E are as defined in (2.30) and (2.23), respectively, the diagonal matrices D_c and D_s are defined by

$$D_c = \mathrm{diag}\,(\cos(\beta_1), \cos(\beta_2), \cos(\beta_3), \cos(\beta_4)) \tag{2.40}$$

and

$$D_s = \mathrm{diag}\,(\sin(\beta_1), \sin(\beta_2), \sin(\beta_3), \sin(\beta_4)), \tag{2.41}$$

and the matrix $\hat{A} \in \mathbb{R}^{4N,4N}$ is in the block partitioned form

$$\hat{A} = \begin{pmatrix} \hat{A}_{1,1} & \hat{A}_{1,2} & \hat{A}_{1,3} & \hat{A}_{1,4} \\ \hat{A}_{2,1} & \hat{A}_{2,2} & \hat{A}_{2,3} & \hat{A}_{2,4} \\ \hat{A}_{3,1} & \hat{A}_{3,2} & \hat{A}_{3,3} & \hat{A}_{3,4} \\ \hat{A}_{4,1} & \hat{A}_{4,2} & \hat{A}_{4,3} & \hat{A}_{4,4} \end{pmatrix}, \tag{2.42}$$

with the elements $\hat{a}_{q,r}^{p,j}$ of the submatrices $\hat{A}_{p,j} \in \mathbb{R}^{N,N}$ $(p, j = 1, 2, 3, 4,)$ being defined in (2.38). With this notation we now prove that:

Lemma 2.3. *The $N \times N$ real submatrices $\hat{A}_{p,j} = \left\{\hat{a}_{q,r}^{p,j}\right\}$, with $\hat{a}_{q,r}^{p,j}$ being as defined in (2.38) satisfy*

$$\hat{A}_{p,j} = \begin{cases} E\hat{A}_0, & p = j \\ -ED\hat{A}_0, & |p-j| = 2 \\ \hat{D}\hat{A}_1, & p-j = -1, 3 \\ \hat{D}\hat{A}_2, & p-j = 1, -3, \end{cases} \tag{2.43}$$

where the elements of the matrix $\hat{A}_0 = \left\{\hat{a}_{q,r}^{(0)}\right\}_{q,r=1}^{N}$ are defined through the Finite Cosine/Sine Fourier Transform of the linear independent real-valued basis functions $\phi_r(s)$, namely

$$\hat{a}_{q,r}^{(0)} = \begin{cases} -\displaystyle\int_{-\pi}^{\pi} \sin\left(\frac{q}{2}s\right)\phi_r(s)\mathrm{d}s, & q = odd \\ \displaystyle\int_{-\pi}^{\pi} \cos\left(\frac{q}{2}s\right)\phi_r(s)\mathrm{d}s, & q = even, \end{cases} \tag{2.44}$$

the elements of the matrix $\hat{A}_1 = \left\{ \hat{a}^{(1)}_{q,r} \right\}_{q,r=1}^{N}$ *are defined by*

$$\hat{a}^{(1)}_{q,r} = \int_{-\pi}^{\pi} \mathrm{e}^{\frac{q}{2}s} \phi_r(s)\mathrm{d}s, \tag{2.45}$$

the elements of the matrix $\hat{A}_2 = \left\{ \hat{a}^{(2)}_{q,r} \right\}_{q,r=1}^{N}$ *are defined by*

$$\hat{a}^{(2)}_{q,r} = (-1)^q \int_{-\pi}^{\pi} \mathrm{e}^{-\frac{q}{2}s} \phi_r(s)\mathrm{d}s, \tag{2.46}$$

the matrices D and E are as defined in Lemma 2.2 and the diagonal matrix $\hat{D}$ *is defined by*

$$\hat{D} = \mathrm{diag}\left(\sin\left(\frac{\pi}{2}\right), \cos\left(2\frac{\pi}{2}\right), \ldots, \sin\left((N-1)\frac{\pi}{2}\right), \cos\left(N\frac{\pi}{2}\right) \right). \tag{2.47}$$

Proof. As in Lemma 2.2, recall the definition of the elements $\hat{a}^{p,j}_{q,r}$ from (2.38) and notice that, for $j = p$, there holds

$$\hat{a}^{p,p}_{q,r} = \mathrm{e}^{l\pi} \begin{cases} -\mathrm{Im}\left(\int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}ls} \varphi_r(s)\mathrm{d}s \right), & l = \frac{1}{2}, \frac{3}{2}, \ldots, \frac{N-1}{2} \\ \mathrm{Re}\left(\int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}ls} \varphi_r(s)\mathrm{d}s \right), & l = 1, 2, \ldots, N/2, \end{cases} \quad q = 2l.$$

Evidently, therefore,

$$\hat{a}^{p,p}_{q,r} = \mathrm{e}^{\frac{q}{2}\pi} \hat{a}^{(0)}_{q,r} \tag{2.48}$$

where $\hat{a}^{(0)}_{q,r}$ are as defined in (2.44), hence

$$\hat{A}_{p,p} = E\hat{A}_0, \quad p = 1, 2, 3, 4. \tag{2.49}$$

Similarly, as $\mathrm{i}^{j-p} = -1$ for $|j - p| = 2$, there holds

$$\hat{a}^{p,j}_{q,r} = \mathrm{e}^{-l\pi} \begin{cases} -\mathrm{Im}\left(\int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}ls} \varphi_r(s)\mathrm{d}s \right) = \int_{-\pi}^{\pi} \sin(ls)\phi_r(s)\mathrm{d}s, & l = \frac{1}{2}, \frac{3}{2}, \ldots, \frac{N-1}{2} \\ \mathrm{Re}\left(\int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}ls} \varphi_r(s)\mathrm{d}s \right) = \int_{-\pi}^{\pi} \cos(ls)\phi_r(s)\mathrm{d}s, & l = 1, 2, \ldots, N/2, \end{cases}$$

with $q = 2l$. Hence, for $|j - p| = 2$,

$$\hat{a}^{p,j}_{q,r} = (-1)^q \mathrm{e}^{-\frac{q}{2}\pi} \hat{a}^{(0)}_{q,r} = -\mathrm{e}^{\frac{q}{2}\pi} \left((-1)^{q-1} \mathrm{e}^{-q\pi} a^{(0)}_{q,r} \right), \tag{2.50}$$

and therefore

$$\hat{A}_{p,j} = -ED\hat{A}_0, \qquad |p - j| = 2. \tag{2.51}$$

Now, as $\mathrm{i}^{j-p} = -i$ for $j - p = -1$ or $j - p = 3$, we have

$$\hat{a}^{p,j}_{q,r} = \left(\int_{-\pi}^{\pi} \mathrm{e}^{ls} \varphi_r(s)\mathrm{d}s \right) \begin{cases} -\mathrm{Im}\left(\mathrm{e}^{-\mathrm{i}l\pi}\right) = \sin(l\pi), & l = \frac{1}{2}, \frac{3}{2}, \ldots, \frac{N-1}{2} \\ \mathrm{Re}\left(\mathrm{e}^{-\mathrm{i}l\pi}\right) = \cos(l\pi), & l = 1, 2, \ldots, N/2, \end{cases}$$

and, therefore,

$$\hat{A}_{p,j} = \hat{D}\hat{A}_1, \quad p - j = -1, 3. \tag{2.52}$$

Finally, as $\mathrm{i}^{j-p} = i$ for $j - p = 1$ or $j - p = -3$, we have

$$\hat{a}^{p,j}_{q,r} = \left(\int_{-\pi}^{\pi} \mathrm{e}^{-ls} \varphi_r(s)\mathrm{d}s \right) \begin{cases} -\mathrm{Im}\left(\mathrm{e}^{il\pi}\right) = -\sin(l\pi), & l = \frac{1}{2}, \frac{3}{2}, \ldots, \frac{N-1}{2} \\ \mathrm{Re}\left(\mathrm{e}^{il\pi}\right) = \cos(l\pi), & l = 1, 2, \ldots, N/2, \end{cases}$$

and, therefore,

$$\hat{A}_{p,j} = \hat{D}\hat{A}_2, \qquad p - j = 1, -3, \tag{2.53}$$

which completes the proof. $\square$

Evidently, therefore, the matrix $\hat{A}$ in (2.42) can be expressed as

$$\hat{A} = (I_4 \otimes E)\tilde{A}_1 + (I_4 \otimes \hat{D})\tilde{A}_2, \tag{2.54}$$

where $\tilde{A}_1$ and $\tilde{A}_2$ denote the block circulant matrices

$$\tilde{A}_1 = \begin{pmatrix} \hat{A}_0 & O & -D\hat{A}_0 & O \\ O & \hat{A}_0 & O & -D\hat{A}_0 \\ -D\hat{A}_0 & O & \hat{A}_0 & O \\ O & -D\hat{A}_0 & O & \hat{A}_0 \end{pmatrix} \quad \text{and} \quad \tilde{A}_2 = \begin{pmatrix} O & \hat{A}_2 & O & \hat{A}_1 \\ \hat{A}_1 & O & \hat{A}_2 & O \\ O & \hat{A}_1 & O & \hat{A}_2 \\ \hat{A}_2 & O & \hat{A}_1 & O \end{pmatrix}. \tag{2.55}$$

If we now let the matrix $\hat{B}$ be defined by

$$\hat{B} = \begin{pmatrix} I & O & -D & O \\ O & I & O & -D \\ -D & O & I & O \\ O & -D & O & I \end{pmatrix}, \tag{2.56}$$

then, upon combination of the results above, we obtain:

Proposition 2.4. *The Collocation coefficient matrix A_C, associated with the linear system described in Proposition 2.3, is expressed as*

$$A_C = (I_4 \otimes E)\left(B(I_4 \otimes A_0)\,(D_c \otimes I_N) + \hat{B}(I_4 \otimes \hat{A}_0)\,(D_s \otimes I_N)\right) + (I_4 \otimes \hat{D})\tilde{A}_2\,(D_s \otimes I_N)\,, \tag{2.57}$$

where the diagonal matrix E and the matrix A_0 are defined in Lemma 2.2, the matrices B and $\hat{B}$ are as defined in (2.31) and (2.56) respectively, the diagonal matrices D_c and D_s are as defined in (2.40) and (2.41) respectively, the matrix $\hat{A}_0$ is defined in Lemma 2.3 and the matrix $\tilde{A}_2$ is as defined in (2.55).

Proof. Recall (2.55) and observe that $\tilde{A}_1 = \hat{B}(I_4 \otimes \hat{A}_0)$. This, combined with relations (2.30), (2.39) and (2.54) yields (2.57) and the proof follows. □

3. Analysis and implementation of numerical methods

Based on the structure, as well as the properties, of the Collocation coefficient matrix, in this section we analyze and implement direct and iterative methods for determining the solution of the generalized Dirichlet–Neumann map associated to Laplace's equation on square domains. For the numerical experiments included, we considered the solution of the model Laplace's equation, with exact solution (cf. [2,3])

$$q(x, y) = \sinh(3x)\sin(3y). \tag{3.1}$$

The relative error E_∞, used to demonstrate the convergence behavior of the direct and iterative methods considered, is given by

$$E_\infty = \frac{\|f - f_N\|_\infty}{\|f\|_\infty}, \tag{3.2}$$

where

$$\|f\|_\infty = \max_{1 \le j \le n} \left\{ \max_{-\pi \le s \le \pi} |f^{(j)}(s)| \right\} \tag{3.3}$$

and

$$\|f - f_N\|_\infty = \max_{1 \le j \le n} \left\{ \max_{-\pi \le s \le \pi} |f^{(j)}(s) - f_N^{(j)}(s)| \right\}, \tag{3.4}$$

with $f_N^{(j)}$ as in (1.7), and the max over s is taken over a dense discretization of the interval $[-\pi, \pi]$. For the direct solution of the linear systems we have used the standard LAPACK routines, while for the computation of the right-hand-side vector we have used a routine (*dqawo*) from QUADPACK implementing the modified Clenshaw–Curtis technique. As it pertains to the iterative methods, the maximum number of iterations, allowed for all methods to perform, is set to 200 and the zero iterate $U^{(0)}$ is set to be equal to the right-hand-side vector. All experiments were conducted on a multi-user SUN V240 system using the Fortran-90 compiler.

Case I: Same boundary conditions on all sides

It is the special sparse structure, revealed in the previous section, of the Collocation system, in (2.29), that allows us to efficiently and rapidly solve it.

Direct solution

Taking advantage of the block structure of the matrix A in (2.30), and observing that the inverse of the matrix B in (2.31) is readily available by

$$B^{-1} = \hat{B}(I_4 \otimes C), \tag{3.5}$$

where $\hat{B}$ is as defined in (2.56) and C is the diagonal matrix

$$C = \operatorname{diag}(c_1, \dots, c_N), \qquad c_q = \frac{1}{1-d_q^2} = \frac{1}{1-\mathrm{e}^{-2q\pi}}, \quad q = 1, \dots, N, \tag{3.6}$$

with d_q denoting the diagonal elements of the matrix D in (2.22), it is evident that the Collocation system (2.29) can be written as

$$(I_4 \otimes A_0)\mathbf{U} = \hat{B}(I_4 \otimes C)(I_4 \otimes E^{-1})\mathbf{G}, \tag{3.7}$$

or, equivalently, as

$$\begin{cases} A_0\mathbf{U}_p = CE^{-1}\left(\mathbf{G}_p - D\mathbf{G}_{p+2}\right), & p = 1, 2 \\ A_0\mathbf{U}_p = CE^{-1}\left(\mathbf{G}_p - D\mathbf{G}_{p-2}\right), & p = 3, 4, \end{cases} \tag{3.8}$$

since the matrices C, D and E are diagonal and commute. The matrix A_0, defined in Lemma 2.2, depends on the choice of basis functions $\varphi_r(s)$, as its elements are defined through their Discrete Cosine/Sine Fourier Transforms (see (2.21)). In [3] we considered the following two choices of basis functions:

(1) *Sine Basis Functions*

$$\varphi_r(s) = \sin\left(r\left(\frac{\pi+s}{2}\right)\right), \quad r = 1, \dots, N. \tag{3.9}$$

(2) *Chebyshev Basis Functions*

$$\varphi_r(s) = \begin{cases} T_{r+1}\left(\dfrac{s}{\pi}\right) - T_0\left(\dfrac{s}{\pi}\right), & r \text{ odd}, \\ T_{r+1}\left(\dfrac{s}{\pi}\right) - T_1\left(\dfrac{s}{\pi}\right), & r \text{ even}, \end{cases} \qquad r = 1, \dots, N, \tag{3.10}$$

where $T_n(x) = \cos\left(n\cos^{-1}(x)\right)$.

For the case of Sine basis functions the matrix A_0 is point diagonal, hence the solution of (3.8) is readily available with computational cost of $\mathcal{O}(N)$. In general, though, including the case of Chebyshev basis functions, it is well known that the computational cost for solving the system (3.8) is $\mathcal{O}(N^3)$, as one has to solve four independent $N \times N$ linear systems with the same coefficient matrix $A_0 \in \mathbb{R}^{N,N}$.

Iterative solution

For an iterative analysis, independent from the choice of basis functions, one may take advantage of the 2-*cyclic* (cf. [9]) nature of the matrix A in (2.30). Observing that its associated *weakly cyclic of index* 2 (cf. [9]) block Jacobi iteration matrix T_0 can be expressed as

$$T_0 = (I_4 \otimes A_0^{-1})(I - B)(I_4 \otimes A_0), \tag{3.11}$$

hence is similar to the matrix

$$I - B = -\begin{pmatrix} O & O & D & O \\ O & O & O & D \\ D & O & O & O \\ O & D & O & O \end{pmatrix} \tag{3.12}$$

where B is as defined in (2.31) and D is the diagonal matrix of (2.22), its spectrum $\sigma(T_0)$ satisfies

$$\sigma(T_0) = \{\pm\mathrm{e}^{-q\pi}, \pm\mathrm{e}^{-q\pi}\}_{q=1}^{N}, \tag{3.13}$$

and, obviously, its spectral radius $\varrho(T_0)$ is given by

$$\varrho(T_0) = \mathrm{e}^{-\pi} \approxeq 0.0432, \tag{3.14}$$

revealing a fast rate of convergence. Moreover, using well known results from the literature (e.g. cf. [9]), the spectral radii of the iteration matrices T_1 and $T_{\omega_{opt}}$, associated to the Gauss–Seidel and the optimal SOR iterative methods, respectively, satisfy

$$\varrho(T_1) = \varrho^2(T_0) = \mathrm{e}^{-2\pi} \approxeq 0.0019, \tag{3.15}$$

and

$$\varrho(T_{\omega_{opt}}) = \omega_{opt} - 1 = \frac{2}{1+\sqrt{1-\mathrm{e}^{-2\pi}}} - 1 \approxeq 0.0005, \tag{3.16}$$

revealing rapid convergence rates. However, we have to point out that, in view of (3.8), the computational cost of the iterative methods is of the same order as that of direct factorization, since for all direct and iterative methods considered the main computational cost comes from the factorization of the matrix A_0. To be more specific, for the solution of the Collocation system in (2.29) or, equivalently, in (3.7) with the change of variables

$$\mathbf{V} = A_0\mathbf{U}, \tag{3.17}$$

the above iterative methods may be implemented through the following expressions:

- *Jacobi*

$$\begin{cases} \mathbf{V}_p^{(m+1)} = -D\mathbf{V}_{p+2}^{(m)} + E^{-1}\mathbf{G}_p, & p = 1, 2 \\ \mathbf{V}_p^{(m+1)} = -D\mathbf{V}_{p-2}^{(m)} + E^{-1}\mathbf{G}_p, & p = 3, 4 \end{cases} \tag{3.18}$$

- *Gauss–Seidel*

$$\begin{cases} \mathbf{V}_p^{(m+1)} = -D\mathbf{V}_{p+2}^{(m)} + E^{-1}\mathbf{G}_p, & p = 1, 2 \\ \mathbf{V}_p^{(m+1)} = -D\mathbf{V}_{p-2}^{(m+1)} + E^{-1}\mathbf{G}_p, & p = 3, 4 \end{cases} \tag{3.19}$$

- *SOR*

$$\begin{cases} \mathbf{V}_p^{(m+1)} = (1-\omega)\mathbf{V}_p^{(m)} - \omega D\mathbf{V}_{p+2}^{(m)} + \omega E^{-1}\mathbf{G}_p, & p = 1, 2 \\ \mathbf{V}_p^{(m+1)} = (1-\omega)\mathbf{V}_p^{(m)} - \omega D\mathbf{V}_{p-2}^{(m+1)} + \omega E^{-1}\mathbf{G}_p, & p = 3, 4. \end{cases} \tag{3.20}$$

Consequently, by also making use of the fast convergence properties of the iterative methods considered, it is apparent that the computational cost, for the iterative solution, is $\mathcal{O}(N)$ for the case of Sine basis functions, while, in general, including the case of Chebyshev basis functions, is $\mathcal{O}(N^3)$ in view of course of (3.17). The idea of an iterative treatment of (3.17) has to be abandoned, at least for the basis functions considered, as for the case of Sine basis functions A_0 is point diagonal while for the case of Chebyshev basis functions A_0 is of low order.

For completeness and uniformity (with the case of different boundary conditions) only purposes, we also consider two of the main representatives from the family of Krylov subspace iterative methods, namely the Bi-CGSTAB [6] and the GMRES [7] methods, for the solution of the preconditioned system

$$AM^{-1}\hat{\mathbf{U}} = (I_4 \otimes E^{-1})\mathbf{G}, \tag{3.21}$$

where, of course, $\hat{\mathbf{U}} = M\mathbf{U}$. Observing that both spectra $\sigma(T_0)$ and $\sigma(T_1) = \sigma^2(T_0)$ of the block Jacobi and block Gauss–Seidel iteration matrices, respectively, are real and *clustered* around zero, it is evident that if we choose the preconditioning matrix M to be the splitting matrix of the Jacobi or the Gauss–Seidel iterative methods, namely

$$M \equiv M_0 = I_4 \otimes A_0 \quad \text{or} \quad M \equiv M_1 = F(I_4 \otimes A_0) \tag{3.22}$$

where

$$F = \begin{pmatrix} I & O & O & O \\ O & I & O & O \\ D & O & I & O \\ O & D & O & I \end{pmatrix}, \tag{3.23}$$

then the spectrum of the preconditioned matrix AM^{-1} would satisfy

$$\sigma\left(AM_0^{-1}\right) = 1 - \sigma(T_0) \quad \text{or} \quad \sigma\left(AM_1^{-1}\right) = 1 - \sigma(T_1), \tag{3.24}$$

since $T_0 = I - M_0^{-1}A$, $T_1 = I - M_1^{-1}A$ and the matrices $M^{-1}A$ and AM^{-1} are obviously similar. Therefore, the eigenvalues of the preconditioned matrices AM_0^{-1} and AM_1^{-1} are all real, located in the half complex plane with the origin being outside or towards the boundary of the convex hull containing them, and clustered around unity. Hence, following [8], the Bi-CGSTAB is expected to have effective convergence properties.

Table 1
Performance of numerical methods (same BC — Chebyshev basis functions)

Method	Preconditioner	$N = 8$			$N = 16$		
		Error	Iter.	Time	Error	Iter.	Time
LU-factorization	–	2.09e−05	–	1.50e−04	5.78e−13	–	2.33e−04
Jacobi	–	2.09e−05	13	2.52e−04	5.78e−13	13	4.74e−04
Gauss–Seidel	–	2.09e−05	7	1.64e−04	5.78e−13	7	2.89e−04
SOR	–	2.09e−05	7	2.05e−04	5.78e−13	7	3.52e−04
Bi-CGSTAB	Jacobi	2.09e−05	2	7.27e−04	5.78e−13	2	8.43e−04
	Gauss–Seidel	2.09e−05	2	7.22e−04	5.78e−13	2	8.37e−04
GMRES(10)	Jacobi	2.09e−05	4	9.21e−04	5.78e−13	4	1.08e−03
	Gauss–Seidel	2.09e−05	3	8.71e−04	5.78e−13	3	1.02e−03

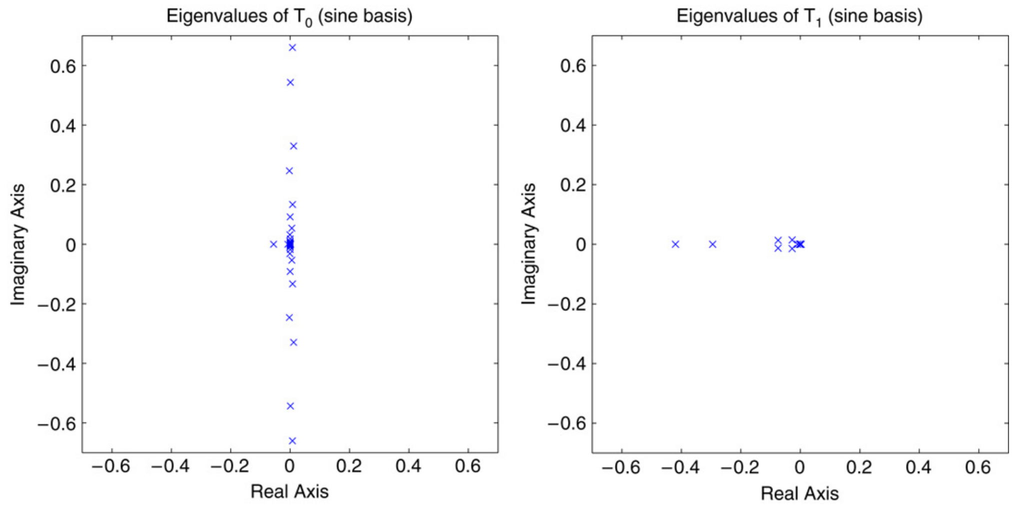

Fig. 1. Eigenvalues of the block Jacobi and GS iteration matrices T_0 and T_1 for Sine basis functions ($N = 64$).

To numerically demonstrate the above results we include Table 1 referring to the performance of all mentioned numerical methods when they apply to the model problem, described at the beginning of this section, for the case of Chebyshev basis functions.

Case II: Different boundary conditions on each side

The numerical treatment, for the case of different boundary conditions on each side of the square domain, largely depends on the boundary conditions used per se. Hence, the numerical results included for this case, are indicative and refer to the mixed boundary conditions (see (2.32)) obtained by making use of the following angles:

$$\beta_1 = \pi, \qquad \beta_2 = \frac{\pi}{4}, \qquad \beta_3 = \frac{\pi}{6}, \qquad \beta_4 = \frac{\pi}{3}.$$

Recall, now, the associated, to the above boundary conditions, Collocation linear system from (2.15), namely

$$A_C\mathbf{U} = \mathbf{G}, \quad A_C \in \mathbb{R}^{4N,4N}, \mathbf{U}, \mathbf{G} \in \mathbb{R}^{4N},$$

where the Collocation matrix A_C is defined in Proposition 2.4 through relation (2.57), and observe that relation (2.39) combined with relation (2.54), contributes to the efficient construction of A_C, as it is written as a matrix combination of circulant matrices, one of which is the matrix A, defined in (2.30), associated to the case of same boundary conditions on all sides of the square.

For Sine basis functions, iterative methods are an effective alternative to direct factorization. This is because, as the Collocation method, combined with the Sine basis functions of (3.9), is quadratically convergent, it is necessary to use a sufficiently large number of basis functions (large N) to achieve a sufficiently small error norm.

To illustrate the convergence behavior of the classical block Jacobi and Gauss–Seidel (GS) methods, with iteration matrices $T_0 = M_0^{-1}N_0$ and $T_1 = M_1^{-1}N_1$ respectively, where

$$M_0 = \bigoplus_{p=1}^{4} M_0^{(p)} \quad \text{with } M_0^{(p)} = E\left(A_0\cos(\beta_p) + \hat{A}_0\sin(\beta_p)\right) \tag{3.25}$$

and M_1 defined analogously, we included Fig. 1 depicting their eigenvalue distribution for a typical case ($N = 64$). Pertaining to the Krylov Bi-CGSTAB and GMRES methods, it is apparent that the use of the un-preconditioned versions is not suggested due to the A_C's eigenvalue distribution depicted in Fig. 2.

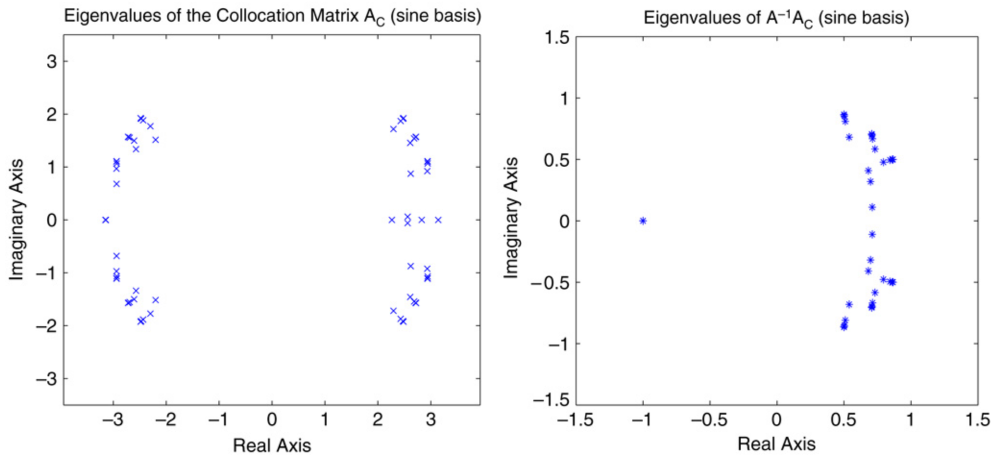

Fig. 2. Eigenvalues of the Matrices A_C and $A^{-1}A_C$ for Sine basis functions ($N = 64$).

Table 2
Performance of numerical methods (different BC — Sine basis functions)

Method	Preconditioner	$N = 32$			$N = 128$			$N = 512$		
		Error	Iter.	Time	Error	Iter.	Time	Error	Iter.	Time
LU-factorization	–	2.05e−03	–	2.29e−02	1.31e−04	–	1.51	7.69e−06	–	192.00
Jacobi	–	2.05e−03	35	2.53e−02	1.31e−04	43	0.76	7.67e−06	53	35.20
GS	–	2.05e−03	16	1.36e−02	1.31e−04	20	0.39	7.69e−06	24	19.30
	Jacobi	2.05e−03	8	1.48e−02	1.31e−04	9	0.51	7.70e−06	9	17.60
Bi-CGSTAB	GS	2.05e−03	4	1.08e−02	1.31e−04	5	0.40	7.69e−06	5	15.30
	A	2.05e−03	29	8.98e−03	1.31e−04	25	0.09	7.62e−06	32	15.00
	Jacobi	2.05e−03	12	1.36e−02	1.31e−04	14	0.47	7.68e−06	16	17.20
GMRES(10)	GS	2.05e−03	7	1.06e−02	1.31e−04	7	0.31	7.70e−06	7	12.70
	A	2.05e−03	37	8.44e−03	1.31e−04	35	0.07	7.67e−06	37	9.18

Table 3
Performance of numerical methods (different BC — Chebyshev basis functions)

Method	Preconditioner	$N = 8$			$N = 12$			$N = 16$		
		Error	Iter.	Time	Error	Iter.	Time	Error	Iter.	Time
LU-factorization	–	4.38e−05	–	5.67e−04	1.45e−08	–	1.37e−03	1.15e−12	–	2.76e−03
Jacobi	–	4.38e−05	66	5.65e−03	1.45e−08	74	9.96e−03	1.16e−12	95	1.93e−02
GS	–	4.38e−05	30	3.16e−03	1.45e−08	34	5.23e−03	1.16e−12	36	8.28e−03
Bi-CGSTAB	Jacobi	4.38e−05	11	2.51e−03	1.45e−08	12	4.12e−03	1.16e−12	13	6.41e−03
	GS	4.38e−05	7	2.27e−03	1.45e−08	7	3.36e−03	1.15e−12	7	4.93e−03
GMRES(10)	Jacobi	4.38e−05	23	3.02e−03	1.45e−08	26	3.89e−03	1.16e−12	28	8.56e−03
	GS	4.38e−05	12	2.39e−03	1.45e−08	13	4.00e−03	1.16e−12	13	5.24e−03

With respect to their preconditioned analogs, together with the block Jacobi and block GS preconditioning, we have also considered the case of using the block circulant matrix A of (2.30) as a preconditioner. Although the eigenvalue distribution of the preconditioned matrix $A^{-1}A_C$ (depicted in Fig. 2) is not that encouraging, the fact that A^{-1} inverse is readily available combined with the large size of the matrices needed to be directly factored out, yields a very efficient preconditioning. In fact, the A-preconditioned GMRES method is significantly less time consuming, hence it is the method of preference. The performance results for all numerical methods considered for the case of Sine basis functions have been included in Table 2.

For the case of Chebyshev basis functions the Collocation method appears to converge exponentially (cf. [3]). Therefore, one may achieve a small error norm with a few basis functions. This fact leads to small size matrices and, therefore, direct factorization is more effective, than iterative methods, for their solution. Nevertheless, for comparison and demonstration purposes, together with the direct factorization method, we also consider the block Jacobi and GS methods, as well as their preconditioning analogs combined with the Bi-CGSTAB and GMRES methods. The eigenvalue distribution of the associated matrices T_0, T_1 and A_C are depicted in Figs. 3 and 4, while the performance results of all numerical methods considered are included in Table 3.

Concluding this paper we would like to remark that there is still a number of very interesting issues, associated with the problem and the methods at hand, that need to be further analyzed. In [5] we have extended our analysis to the case of regular polygon domains with arbitrary number of vertices. However, the analysis of general polygon domains remains an

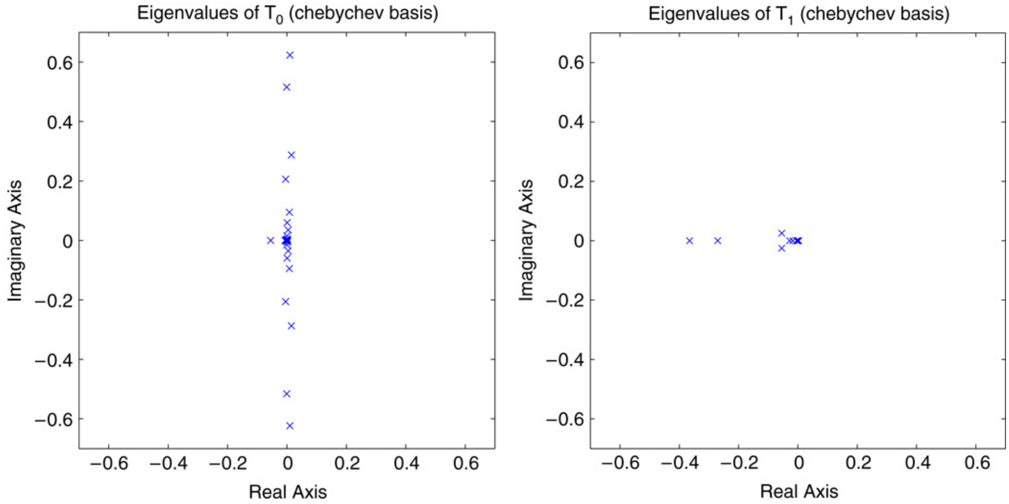

Fig. 3. Eigenvalues of the block Jacobi and GS iteration matrices T_0 and T_1 for Chebyshev basis functions ($N = 16$).

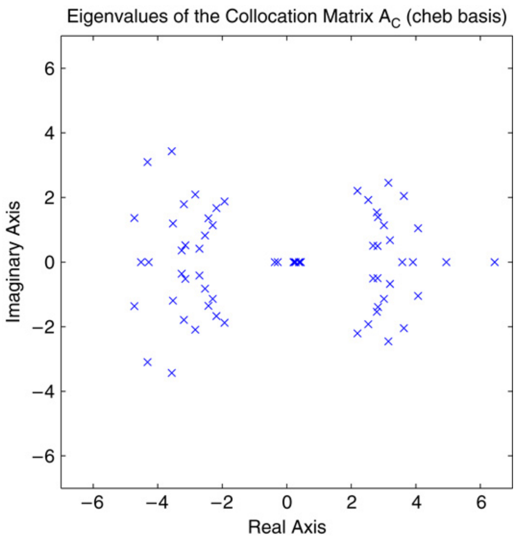

Fig. 4. Eigenvalues of the Collocation Matrix A_C of (2.57) for Chebyshev basis functions ($N = 16$).

open problem and it is premature, for the time being, to risk general conclusions. Applications involving general polygon domains with low number of vertices form a particularly interesting and, possibly, analytically feasible problem to solve.

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