

Numerical Study of Iterative Methods for the Solution of the Dirichlet-Neumann Map for Linear Elliptic PDEs on Regular Polygon Domains

A. G. Sifalakis and E. P. Papadopoulou and Y. G. Saridakis

Abstract—A generalized Dirichlet to Neumann map is one of the main aspects characterizing a recently introduced method for analyzing linear elliptic PDEs, through which it became possible to couple known and unknown components of the solution on the boundary of the domain without solving on its interior. For its numerical solution, a well conditioned quadratically convergent sine-Collocation method was developed, which yielded a linear system of equations with the diagonal blocks of its associated coefficient matrix being *point diagonal*. This structural property, among others, initiated interest for the employment of iterative methods for its solution. In this work we present a conclusive numerical study for the behavior of classical (Jacobi and Gauss-Seidel) and Krylov subspace (GMRES and Bi-CGSTAB) iterative methods when they are applied for the solution of the Dirichlet to Neumann map associated with the Laplace's equation on regular polygons with the same boundary conditions on all edges.

Keywords—Elliptic PDEs, Dirichlet to Neumann Map, Global Relation, Collocation, Iterative Methods, Jacobi, Gauss-Seidel, GMRES, Bi-CGSTAB.

I. INTRODUCTION

A New approach for analyzing boundary value problems for linear and for integrable nonlinear PDEs in two dimensions was introduced in [1] and [4]. This approach characterizes a generalized Dirichlet to Neumann map through the solution of the so-called *global relation*, namely, an equation, valid for all values

Manuscript received May 10, 2007. This work was supported by the Greek Ministry of Education "Herakleitos" EPEAEK Grant which is partially supported by the EU

A. G. Sifalakis is with the Department of Sciences, Technical University of Crete, University Campus, 73100 Chania, Greece (e-mail: sifal@science.tuc.gr).

E. P. Papadopoulou is with the Department of Sciences, Technical University of Crete, University Campus, 73100 Chania, Greece (e-mail: elena@science.tuc.gr)

Y. G. Saridakis is with the Department of Sciences, Technical University of Crete, University Campus, 73100 Chania, Greece (phone: +30-28210-37740; fax: +30-28210-37842; e-mail: yiannis@science.tuc.gr).

of a complex parameter k , coupling specified known and unknown values of the solution and its derivatives on the boundary.

For a large class of boundary value problems, the global relation can be solved analytically (see e.g. [4]-[6]), and hence the generalized Dirichlet to Neumann map can be constructed in closed form. However, for general boundary value problems, the global relation must be solved numerically.

The implementation of the new method to the case of the Laplace equation in an arbitrary bounded convex polygon was presented in [2], where a Sine-Collocation type numerical method was also introduced. In [3], we introduced a new set of *Collocation points* which yielded a well-conditioned quadratically convergent Sine-Collocation method. Moreover, the diagonal blocks of the associated coefficient matrix of the corresponding linear system were diagonal matrices. That is, the collocation coefficient matrix is by construction *block-Jacobi preconditioned*, pointing directly to the efficient implementation of iterative techniques. The first indicative numerical results, included in [3], relevant to the behavior of certain iterative methods, provided further support to this argument.

In the work herein, we present a conclusive numerical study for the behavior of the classical Jacobi and Gauss-Seidel as well as the GMRES[7] and the Bi-CGSTAB[8] iterative techniques applied to the solution of the model Dirichlet to Neumann map related to the Laplace's equation on several regular polygons with the same boundary conditions on all edges. We concluded that, while for polygons with small number of edges all methods converge rapidly, the Bi-CGSTAB method is the method of choice as it converges always faster in all cases of polygons independently of the number of edges, the number of basis functions and the boundary conditions.

The paper is organized as follows: Section 2 outlines some of the analytical results of [2] and [3] together

with the construction of the related Collocation linear system. Section 3 presents the numerical study for the behavior of the iterative methods considered.

II. OVERVIEW

To fix notation (see [2], [3]), let us consider the complex form of Laplace's equation in the independent variable q

$$\frac{\partial^2 q}{\partial z \partial \bar{z}} = 0. \tag{1}$$

The above equation is equivalent to the equation

$$\frac{\partial}{\partial \bar{z}} \left(e^{-ikz} \frac{\partial q}{\partial z} \right) = 0 \tag{2}$$

for an arbitrary complex parameter k . Suppose, now, that the real-valued function $q(z, \bar{z})$ satisfies Laplace's equation (1) in a simply connected bounded domain D with boundary ∂D . Then, equation (2), combined with the complex form of Green's theorem implies the equation

$$\int_{\partial D} e^{-ikz} \frac{\partial q}{\partial z} dz = 0, \quad k \in \mathbb{C}. \tag{3}$$

Equation (3) is referred to as the *global relation* associated with Laplace's equation. If we now consider the case of D being a convex bounded polygon with vertices z_1, z_2, \dots, z_n (modulo n) have been indexed counter-clockwise (see Fig. 1), then the global relation (3) becomes

$$\sum_{j=1}^n \int_{S_j} e^{-ikz} \frac{\partial q}{\partial z} dz = 0, \quad k \in \mathbb{C}, \tag{4}$$

where S_j denotes the side from z_j to z_{j+1} (not including the end points).

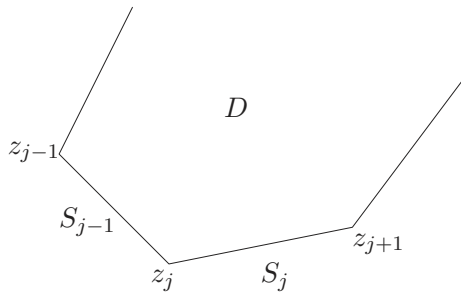


Fig. 1. Part of the bounded convex polygon with vertices z_j , sides S_j , and interior D .

Let, now, for $z \in S_j, 1 \leq j \leq n$,

- $g^{(j)}$ denote the derivative of the solution in the direction making an angle $\beta_j, 0 \leq \beta_j \leq \pi$ with the side S_j , i.e.

$$\cos(\beta_j) q_s^{(j)} + \sin(\beta_j) q_n^{(j)} = g^{(j)},$$

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

$$-\sin(\beta_j) q_s^{(j)} + \cos(\beta_j) q_n^{(j)} = f^{(j)},$$

where $q_s^{(j)}$ and $q_n^{(j)}$ denote the tangential and (outward) normal components of $\frac{\partial q}{\partial z}$ along the side S_j . For $z \in S_j$ and $-\pi < s < \pi$, with

$$z = \frac{1}{2} (z_j + z_{j+1}) + \frac{s}{2\pi} (z_{j+1} - z_j),$$

the *Generalized Dirichlet-Neumann map*, that is the relation between the sets $\{f^{(j)}(s)\}_{j=1}^n$ and $\{g^{(j)}(s)\}_{j=1}^n$, is characterized by the single equation

$$\sum_{j=1}^n |h_j| e^{i(\beta_j - km_j)} \cdot \int_{-\pi}^{\pi} e^{-ikh_j s} (f^{(j)} - ig^{(j)}) ds = 0, \quad k \in \mathbb{C} \tag{5}$$

where, for $j = 1, 2, \dots, n$,

$$h_j := \frac{1}{2\pi} (z_{j+1} - z_j), \tag{6}$$

$$m_j := \frac{1}{2} (z_{j+1} + z_j), \tag{7}$$

and $z_{n+1} = z_1$. Evaluating equation (5) on the following n -rays of the complex k -plane

$$k_p = -\frac{l}{h_p}, \quad l \in \mathbb{R}^+, \quad p = 1, \dots, n \tag{8}$$

and multiplying the resulting equations by $\exp[-i(\beta_p + lm_p/h_p)] / |h_p|$, equation (5) yields the following set of n equations (cf. [2]):

$$\sum_{j=1}^n \frac{|h_j|}{|h_p|} e^{i(\beta_j - \beta_p)} e^{-\frac{il}{h_p}(m_p - m_j)} \cdot \int_{-\pi}^{\pi} e^{il \frac{h_j}{h_p} s} (f^{(j)} - ig^{(j)}) ds = 0, \tag{9}$$

for $p = 1, \dots, n$.

Suppose that the set $\{g^{(j)}(s)\}_{j=1}^n$ is given, and that $\{f^{(j)}(s)\}_{j=1}^n$ is approximated by $\{f_N^{(j)}(s)\}_{j=1}^n$ where

$$f_N^{(j)}(s) = f_*^{(j)}(s) + \sum_{r=1}^N U_r^j \varphi_r(s) \tag{10}$$

with N being an even integer, and

$$2\pi f_*^{(j)}(s) = (s + \pi) f^{(j)}(\pi) - (s - \pi) f^{(j)}(-\pi) . \tag{11}$$

Note that the values of $f^{(j)}(\pi)$ and $f^{(j)}(-\pi)$ can be computed by the continuity requirements at the vertices of the polygon. The set of functions $\{\varphi_r(s)\}_{r=1}^N$ are the *basis* functions which, for the purpose of this paper, are constructed from the Sine functions; namely

$$\varphi_r(s) = \sin(r \frac{\pi + s}{2}) \tag{12}$$

Then, the real coefficients U_r^j satisfy the $(Nn) \times (Nn)$ system of linear algebraic equations (cf. [3])

$$\sum_{j=1}^n \frac{|h_j|}{|h_p|} e^{i(\beta_j - \beta_p)} e^{-i \frac{l}{h_p} (m_p - m_j)} \cdot \sum_{r=1}^N U_r^j \int_{-\pi}^{\pi} e^{i l \frac{h_j}{h_p} s} \varphi_r(s) ds = G_p(l) \tag{13}$$

where $G_p(l)$ denotes the known function

$$G_p(l) = i \sum_{j=1}^n \frac{|h_j|}{|h_p|} e^{i(\beta_j - \beta_p)} e^{-i \frac{l}{h_p} (m_p - m_j)} \cdot \int_{-\pi}^{\pi} U_r^j e^{i l \frac{h_j}{h_p} s} \left(g^{(j)}(s) + i f_*^{(j)}(s) \right) ds \tag{14}$$

and l is chosen as follows:

- For the real part of equations (13) ,

$$l = \frac{1}{2}, \frac{3}{2}, \dots, \frac{N-1}{2}$$

- For the imaginary part of equations (13)

$$l = 1, 2, \dots, N/2 .$$

It was the choice of the aforementioned collocation points (defined by the choice of the parameter l) that lead us to a well conditioned *point diagonal* collocation matrix, shown schematically in Fig. 2. The, numerically observed, convergence rate of the method is quadratic [3] and as the matrix is, by default, *Block Jacobi Preconditioned*, iterative methods appear to be a natural choice for the solution of the corresponding collocation system.

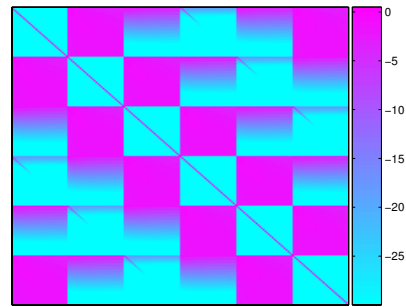


Fig. 2. The structure of the collocation coefficient matrix for $n = 6$ and $N = 32$

III. NUMERICAL STUDY OF ITERATIVE METHODS

In this section we have included results, from the numerical study conducted, pertaining to the behavior of iterative methods for the class of Laplace's problems having the same boundary conditions on all polygon's edges. For this class, following the analysis included in section II and particularly equation (13), which describes the linear system under consideration, one may easily verify that the Collocation coefficient matrix depends only on the choice and the number of the basis functions as well as on the number of the polygon's edges, while at the same time remains independent from the form of the boundary conditions and the form of the exact solution of Laplace's equation. Therefore, the numerical study focuses on the convergence behavior of iterative methods with respect to the number of vertices and the number of basis functions. However, for the sake of completeness, we have included experiments of all kind of boundary conditions for different polygon sizes. For simplicity and space economy, the results included here are related to a model Laplace equation with exact solution ([2], [3])

$$q(x, y) = \sinh(3x) \sin(3y) . \tag{15}$$

We are pointing out once more, that all iterative methods behave similarly in all cases of problems of this class with Dirichlet ($\beta_j = 0$), Neumann ($\beta_j = \pi/2$) or Mixed ($\beta_j = \pi/3$) boundary conditions. The relative error E_∞ , used to demonstrate the convergence behavior of the iterative methods, is given by

$$E_\infty = \frac{\|f - f_N\|_\infty}{\|f\|_\infty} , \tag{16}$$

where

$$\|f\|_\infty = \max_{1 \leq j \leq n} \left\{ \max_{-\pi \leq s \leq \pi} |f^{(j)}(s)| \right\} \quad (17)$$

and

$$\|f - f_N\|_\infty = \max_{1 \leq j \leq n} \left\{ \max_{-\pi \leq s \leq \pi} |f^{(j)}(s) - f_N^{(j)}(s)| \right\}, \quad (18)$$

with $f_N^{(j)}$ as in (10), 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. Apart from the classical Jacobi and Gauss-Seidel methods we have also considered the representative Krylov GMRES(10) and Bi-CGSTAB methods in two forms : (a) the unpreconditioned form or, equivalently, the block Jacobi preconditioned, due to the structure of the collocation matrix, and (b) the Symmetric Gauss-Seidel (SGS) preconditioned form, a two sided preconditioning method derived from the Symmetric SOR preconditioner for $\omega = 1$. The maximum number of iterations, allowed for all methods to perform, is set to 200 and the tolerance for the stopping criteria in all methods is set to 10^{-6} . The zero iterate $U^{(0)}$ is set to be equal to the right hand side vector. The results we have included refer to the representative cases of regular polygons with 8, 12, 19, 24, 31 and 36 edges. All polygons are constructed as in [3]. All experiments were conducted on a multiuser SUN V880 system using the Fortran-90 compiler.

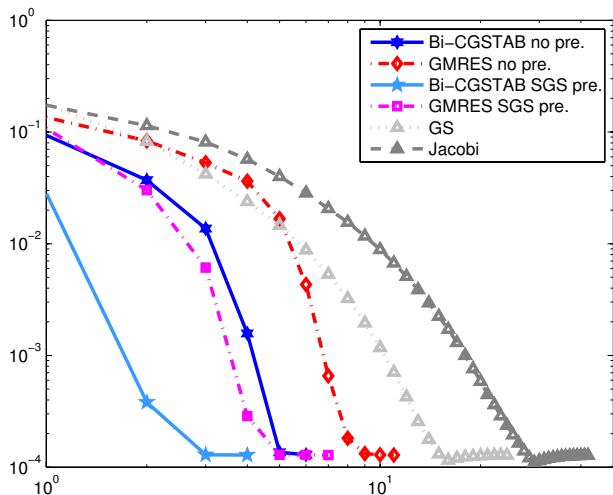


Fig. 1 : 8-gon/Dirichlet BC : Reduction of E_∞ vs Iterations ($N = 32$)

TABLE I
REGULAR OCTAGON / DIRICHLET BC : NUMBER OF ITERATIONS

N	Jacobi	Gauss-Seidel	GMRES		Bi-CGSTAB	
			unpre	pre	unpre	pre
8	40	24	10	6	6	3
16	41	24	10	6	6	3
32	42	24	11	7	6	4
64	42	25	12	7	6	5

TABLE II
REGULAR OCTAGON / DIRICHLET BC : TIME (SEC $\times 10^{-2}$)

N	LU	Jacobi	Gauss-Seidel	GMRES		Bi-CGSTAB	
				unpre	pre	unpre	pre
8	0.6	2.1	1.0	0.4	0.6	0.5	0.5
16	4.5	4.7	2.6	1.3	1.7	1.4	1.7
32	40.6	13.9	8.5	5.8	9.3	4.85	12.4
64	414	105	34	31	30	24	39

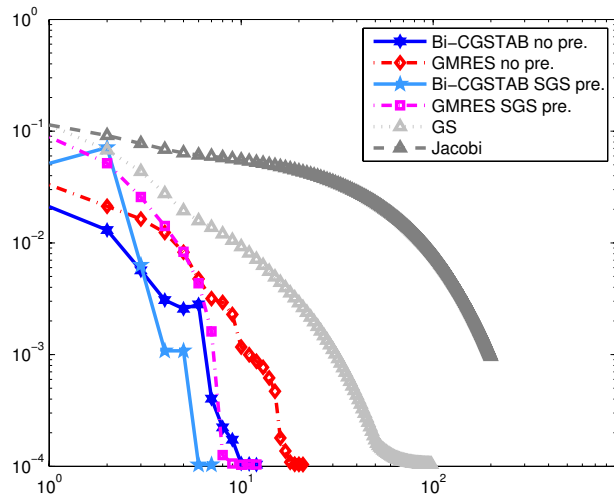


Fig. 2 : 12-gon/Dirichlet BC : Reduction of E_∞ vs Iterations ($N = 32$)

TABLE III
REGULAR 12-GON / DIRICHLET BC : NUMBER OF ITERATIONS

N	Jacobi	Gauss-Seidel	GMRES		Bi-CGSTAB	
			unpre	pre	unpre	pre
8	200	87	19	12	10	7
16	200	94	21	12	10	7
32	200+	98	21	12	12	7
64	200+	100	21	13	11	7

TABLE IV
REGULAR 12-GON / DIRICHLET BC : TIME (SEC $\times 10^{-2}$)

N	LU	Jacobi	Gauss-Seidel	GMRES		Bi-CGSTAB	
				unpre	pre	unpre	pre
8	1.95	22.5	7.59	1.33	1.99	1.24	1.84
16	15.8	51.1	22.1	6.0	6.3	4.0	6.7
32	135	152	78	23	27	22	28
64	1450	1360	739	239	267	222	271

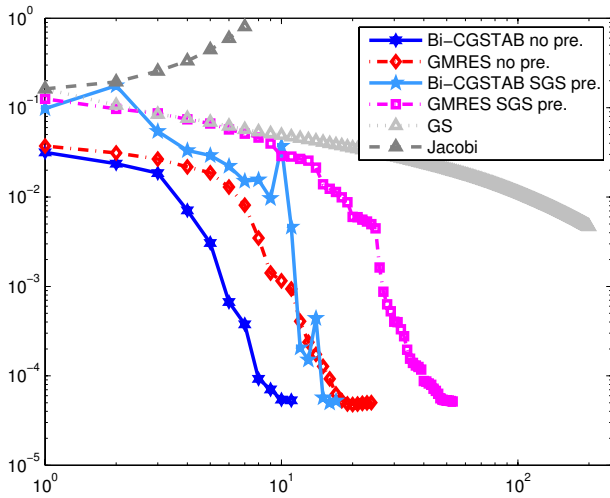


Fig. 3 : 19-gon/Neumann BC : Reduction of E_∞ vs Iterations ($N = 32$)

TABLE V

REGULAR 19-GON / NEUMANN BC : NUMBER OF ITERATIONS

N	Jacobi	Gauss-Seidel	GMRES		Bi-CGSTAB	
			unpre	pre	unpre	pre
8	div	200+	20	37	11	14
16	div	200+	23	53	11	16
32	div	200+	24	53	11	17
64	div	200+	24	52	11	19

TABLE VI

REGULAR 19-GON / NEUMANN BC : TIME (SEC)

N	LU	Jacobi	Gauss-Seidel	GMRES		Bi-CGSTAB	
				unpre	pre	unpre	pre
8	0.08	-	>0.44	0.03	0.12	0.03	0.08
16	0.66	-	>1.18	0.16	0.65	0.12	0.35
32	5.46	-	>4.33	0.76	2.86	0.67	1.68
64	159	-	>92.9	14.4	59.5	12.5	42.9

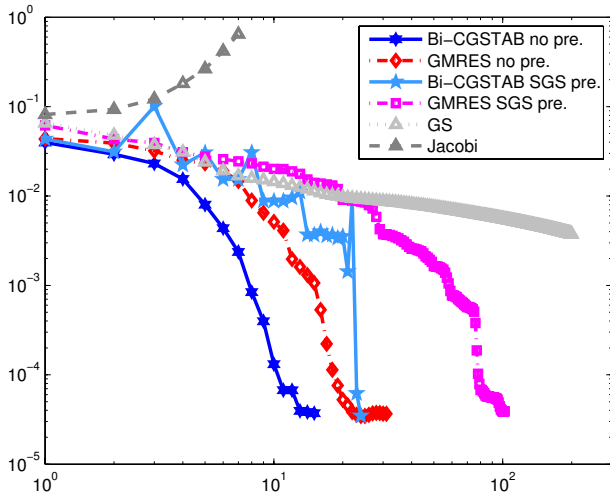


Fig. 4 : 24-gon/Dirichlet BC : Reduction of E_∞ vs Iterations ($N = 32$)

TABLE VII

REGULAR 24-GON / DIRICHLET BC : NUMBER OF ITERATIONS

N	Jacobi	Gauss-Seidel	GMRES		Bi-CGSTAB	
			unpre	pre	unpre	pre
8	div	200+	28	50	15	21
16	div	200+	29	78	14	25
32	div	200+	31	102	15	24
64	div	200+	32	114	16	25

TABLE VIII

REGULAR 24-GON / DIRICHLET BC : TIME (SEC)

N	LU	Jacobi	Gauss-Seidel	GMRES		Bi-CGSTAB	
				unpre	pre	unpre	pre
8	0.2	-	>0.72	0.07	0.25	0.06	0.19
16	1.37	-	>2.00	0.28	1.71	0.24	0.95
32	17.6	-	>16.8	3.67	21.6	3.61	10.7
64	323	-	>134	27.4	183	26.0	80.5

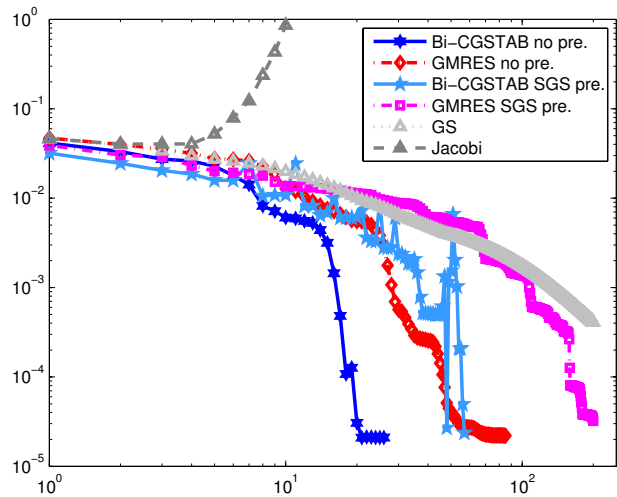


Fig. 5 : 31-gon / Mixed BC : Reduction of E_∞ vs Iterations ($N = 32$)

TABLE IX

REGULAR 31-GON / MIXED BC : NUMBER OF ITERATIONS

N	Jacobi	Gauss-Seidel	GMRES		Bi-CGSTAB	
			unpre	pre	unpre	pre
8	div	200+	91	103	23	44
16	div	200+	89	157	31	53
32	div	200+	85	200+	24	57
64	div	200+	87	200+	28	59

TABLE X

REGULAR 31-GON / MIXED BC : TIME (SEC)

N	LU	Jacobi	Gauss-Seidel	GMRES		Bi-CGSTAB	
				unpre	pre	unpre	pre
8	0.35	-	>1.17	0.36	0.83	0.14	0.64
16	2.96	-	>3.2	1.56	5.38	0.95	3.38
32	66.3	-	>61.1	33.0	>144	16.0	69.1
64	909	-	>271	144	>635	84.2	345

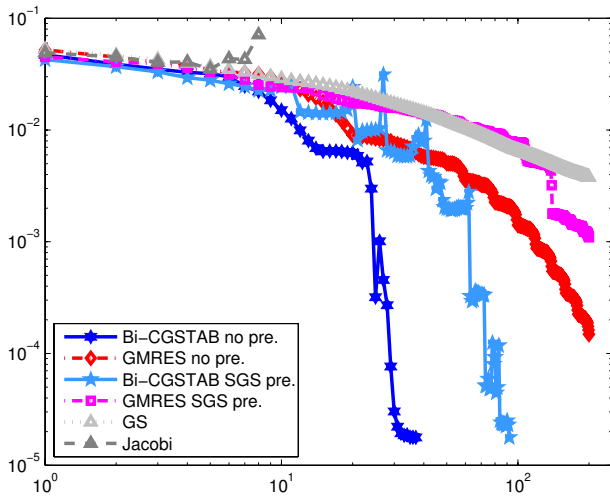


Fig. 6 : 36-gon/Dirichlet BC : Reduction of E_{∞} vs Iterations ($N = 32$)

TABLE XI

REGULAR 36-GON / DIRICHLET BC : NUMBER OF ITERATIONS

N	Jacobi	Gauss-Seidel	GMRES		Bi-CGSTAB	
			unpre	pre	unpre	pre
8	div	200+	200+	200+	33	68
16	div	200+	200+	200+	35	76
32	div	200+	200+	200+	37	93
64	div	200+	200+	200+	37	95

TABLE XII

REGULAR 36-GON / DIRICHLET BC : TIME (SEC)

N	LU	Jacobi	Gauss-Seidel	GMRES		Bi-CGSTAB	
				unpre	pre	unpre	pre
8	0.6	-	>1.6	>1.1	>2.2	0.3	1.4
16	4.7	-	>4.7	>5.4	>10.4	1.6	7.0
32	133	-	>87	>105	>200	35	178
64	1300	-	>322	>389	>748	134	695

Figure 1 and Tables I and II summarize the results pertaining to the case of a Regular Octagon, a representative case for polygons with relatively *small* number of edges (triangles, squares, pentagons, hexagons, etc). Inspecting these data one may easily observe that :

- All methods converge smoothly in a few iterations
- The convergence rate of the Bi-CGSTAB method is faster than all other iterative methods
- Preconditioning improves the rate of convergence but increases the computational cost
- The convergence rate remains independent of N
- LU-factorization competes with the iterative methods only for small N .

As, now, the number of edges increases we observe that (see Fig. 2-6 and Tables III-XII):

- The Jacobi method diverges for polygons with medium and large number of edges
- The Gauss-Seidel method converges smoothly but very slowly
- The un-preconditioned versions of both Krylov methods converge smoothly
- The un-preconditioned version of the GMRES method fails to converge within 200 iterations for the case of the regular 36-gon
- The un-preconditioned Bi-CGSTAB converged in all experiments rapidly and its convergence rate remained faster than the un-preconditioned GMRES and the two classical iterative methods
- The SGS preconditioner for polygons with medium and large number of edges did not improve the convergence rate of both the Krylov methods and increased in all cases the computational cost
- The Krylov methods (except GMRES for the case of the 36-gon) are spectacularly more efficient than LU-factorization.

In conclusion, the un-preconditioned version of the Bi-CGSTAB is the most efficient and safe method to be employed for the solution of the linear system arising from the solution of the Dirichlet to Neumann map associated with the Laplace equation on regular polygons with the same Dirichlet, Neumann or Mixed Boundary Conditions on all edges. A spectral analysis for the theoretical justification of these results is under development.

- [1] A.S.Fokas, A unified transform method for solving linear and certain nonlinear PDEs, *Proc. R. Soc. London A* **53** (1997), 1411-1443.
- [2] S. Fulton, A.S. Fokas and C. Xenophontos, An Analytical Method for Linear Elliptic PDEs and its Numerical Implementation, *J. of CAM* **167** (2004), 465-483.
- [3] A. Sifalakis, A.S. Fokas, S. Fulton and Y.G. Saridakis, The Generalized Dirichlet-Neumann Map for Linear Elliptic PDEs and its Numerical Implementation, *J. of Comput. and Appl. Maths.* (in press)
- [4] A.S.Fokas, Two-dimensional linear PDEs in a convex polygon, *Proc. R. Soc. London A* **457** (2001), 371-393.
- [5] A.S. Fokas, A New Transform Method for Evolution PDEs, *IMA J. Appl. Math.* **67** (2002), 559.
- [6] G. Dassios and A.S. Fokas, The Basic Elliptic Equations in an Equilateral Triangle, *Proc. R. Soc. Lond. A* **461** (2005), 2721-2748.
- [7] Y. Saad and M. Schultz, GMRES: a generalized minimal residual algorithm for solving nonsymmetric linear systems, *SIAM J. Sci. Statist. Comput.*, **7**, 1986, pp. 856-869.
- [8] H.A. Van Der Vorst, Bi-CGSTAB: A fast and smoothly converging variant of Bi-CG for the solution of nonsymmetric linear systems, *SIAM J. Sci. Statist. Comput.*, **13**, 1992, pp. 631-644.