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Splitting methods for solving singular linear systems of a special class

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RIASSUNTO: In questo lavoro consideriamo una classe speciale di sistemi lineari singolari provenienti dalla discretizzazione di una equazione ellittica del secondo ordine con condizione al contorno di tipo derivata obliqua. Per risolvere numericamente tali sistemi si propone di utilizzare il metodo degli spostamenti simultanei con un precondizionatore additivo; questo metodo é particolarmente adatto ad essere realizzato su calcolatori multivettoriali. Si analizza la convergenza di siffatto metodo, fornendo una condizione sufficiente di convergenza per valori "piccoli" del fattore di rilassamento. Alcuni esperimenti numerici su problemi rappresentativi confermano i risultati teorici e mostrano l'efficienza del metodo.

ABSTRACT: This paper is concerned with the solution of singular linear systems of a special class which arise in discretizing a linear elliptic equation of the second-order with an oblique-derivative type boundary condition. We propose to solve these systems with the Method of Simultaneous Displacements with the additive preconditioner: this method is ideally suited for implementation on multivector computers. The convergence of such a method has been analysed and a sufficient convergence-criterion has been established.

Generally, only for small values of the relaxation factor the method is convergent. The numerical results obtained by solving some test-problems are seen to be largely in keeping with the theory and show the effectiveness of the method.

KEY WORDS AND PHRASES: Large scale linear systems – Iterative methods – Singular systems

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1 – Introduction

The classical Poincarè Problem, formulated in connection with the study of tidal motions [5], reduces to solving a linear elliptic equation of the second-order with an oblique-derivative type boundary condition. Analogous problems arise in determining the deviations of the reference surface of the ocean due to large-scale currents and in solving the equations of the baroclinic ocean by the method of orthogonal expansions.

Numerical solution of the Poincarè Problem involves certain difficulties associated with the selection of suitable approximations of boundary conditions [1], [4], [6]. The papers [1], [4] employ Stommel's model [7] of ocean circulation for examining a method of numerical solution of the problem with oblique-derivative: algebraic equations for this model are obtained by the finite difference method. In particular, in [1] a suitable finite difference approximation to the continuous problem has been obtained in order to produce a discrete matrix equation which satisfies the basic properties of the continuous problem.

This discrete matrix equation can be written in the form

(1)
$$(A+B)\mathbf{u} = \mathbf{f}$$

where $\mathbf{u}, \mathbf{f} \in \mathbb{R}^n, A = (a_{ij})$ is an $n \times n$ real, irreducible, symmetric and positive semidefinite matrix, $B = (b_{ij})$ is an $n \times n$ real and skew-symmetric matrix, A + B is irreducible and singular:

(2) $A = A^T$ positive semidefinite, $B = -B^T$, det(A + B) = 0.

Furthermore, we have that:

• the sum of the entries of any row of A and of B is equal to zero:

(3)
$$A\mathbf{e} = 0, \quad B\mathbf{e} = 0 \text{ where } \mathbf{e} = (1, 1, \dots, 1)^T,$$

that is, **e** is an eigenvector of A, $A^T(=A)$, B, $B^T(=-B)$, A+B and $(A+B)^T(=A-B)$, corresponding to the zero eigenvalue;

• the diagonal entries of A are positive and the nondiagonal entries of A are non positive:

(4)
$$a_{ii} > 0, \quad a_{ij} \le 0 \quad i \ne j;$$

• for any real constant c > 0, the matrix A + cI is non singular and the entries of its inverse are positive (i.e., A + cI is an M-matrix):

(5)
$$\det(A+cI) > 0, \quad (A+cI)^{-1} > 0 \text{ with } c > 0.$$

We assume that (1) is solvable, that is, $\mathbf{f} \in \mathcal{R}(A+B)$, where $\mathcal{R}(A+B)$ denotes the range of A+B, or \mathbf{f} is orthogonal to the null space of $(A+B)^T$.

This paper is concerned with the development of the Method of Simultaneous Displacements with the additive preconditioner for solving the special linear system (1) when the coefficient matrix A + B is a large, sparse matrix which satisfies the conditions (2)-(5). This method is ideally suited for implementation on a multiprocessor system with two or more vector processors, such as the CRAY Y-MP. The Method of Simultaneous Displacements with the additive preconditioner has been studied in [2] for large classes of singular matrices arising from the discretization with finite difference formulas of elliptic problems. However, for the elliptic problem considered in this paper (section 4) it was necessary to perform a deeper analysis of the coefficient matrix of (1). Our principal aim was to construct a suitable finite difference approximation of the continuous problem which produces a matrix equation satisfying the basic properties of the continuous problem. This special coefficient matrix does not belong to the classes of coefficient matrices considered in [2]. Also in this case the method is convergent; in section 3 a sufficient convergencecriterion has been established. Generally, only for small values of the relaxation factor ω the method is convergent. The numerical results obtained by solving some test-problems are seen to be largely in keeping with the theory and show the effectiveness of the method.

2 – Some properties of the coefficient matrix

In this section we state some properties of the coefficient matrix of system (1).

LEMMA 1. Assume that (2)-(5) hold. Then,

 (i) the vector e, defined in (3), is the unique (up to a scalar multiple) eigenvector of A and of A + B corresponding to the zero eigenvalue;

(ii) the zero eigenvalue is a simple eigenvalue of A and of A + B.

PROOF. Part (i): from (5) it follows that \mathbf{e} is the unique (up to a constant multiple) eigenvector of (A+cI) corresponding to the eigenvalue c > 0: $(A+cI)\mathbf{e} = c\mathbf{e}$. Therefore, if there exists a vector $\mathbf{e}' \neq 0$ such that $A\mathbf{e}' = 0$ and $\mathbf{e}' \neq \mathbf{e}$, then we would have that $(A + cI)\mathbf{e}' = c\mathbf{e}'$, which contradicts the uniqueness of \mathbf{e} . Assume now that there exists a vector $\mathbf{e}' \neq \mathbf{e}$ such that $(A + B)\mathbf{e}' = 0$. Since B is skew-symmetric, i.e. the inner product $(\mathbf{e}', B\mathbf{e}') = -(\mathbf{e}', B\mathbf{e}')$, we obtain $(\mathbf{e}', A\mathbf{e}') = 0$. From the previous argument it follows that $\mathbf{e}' = \mathbf{e}$.

Part (ii): for the symmetric matrix A, part (i) implies part (ii). The proof of part (ii) for the matrix A+B is based on the fact that \mathbf{e} is unique (apart from a nonzero scalar multiplier) eigenvector, corresponding to the zero eigenvalue, of both A+B and of its transpose A-B. For the matrix A+B, part (i) implies that in the Jordan canonical form of the matrix A+B there is only one Jordan canonical box with zero diagonal entries. Let λ^m , $m \geq 1$, be the elementary divisor corresponding to this box. To this elementary divisor there corresponds a definite cyclic subspace I_0 , generated by a vector which we denote by \mathbf{e}_0 . For this vector λ^m is the minimal polynomial. We consider the Krylov vectors [3, pg. 200]

$$\mathbf{e}_1 = (A+B)^{m-1}\mathbf{e}_0, \ \mathbf{e}_2 = (A+B)^{m-2}\mathbf{e}_0, \dots$$

and we note that

$$(A+B)\mathbf{e}_1 = (A+B)^m \mathbf{e}_0 = 0, \ (A+B)\mathbf{e}_2 = (A+B)^{m-1}\mathbf{e}_0 = \mathbf{e}_1.$$

From part (i) we have that $\mathbf{e}_1 = \mathbf{e}$. If $m \ge 2$, then we would have $(A+B)\mathbf{e}_2 = \mathbf{e}$ and consequently $((A-B)\mathbf{e},\mathbf{e}_2) = \|\mathbf{e}\|^2 = 0$, which would imply $\mathbf{e} = 0$. Thus, m = 1 (the elementary divisor is linear) and the zero eigenvalue of A + B is simple.

Notice that if \mathbf{u}^* is a solution of (1) so is $\mathbf{u}^* + \gamma \mathbf{e}$, for any real γ ; moreover, because of Lemma 1, all solutions of (1) have this form.

From Lemma 1, it follows that the solvability condition of the singular system (1) is given by

(6)
$$(\mathbf{f}, \mathbf{e}) = (\mathbf{u}, (A+B)^T \mathbf{e}) = (\mathbf{u}, 0) = 0$$

where (\mathbf{f}, \mathbf{e}) is the inner product of \mathbf{f} and \mathbf{e} .

LEMMA 2. Assume that (2)-(5) hold. Let D be the diagonal matrix with the same diagonal entries of A and let μ be any eigenvalue of $D^{-1}(A+B)$. Then, $\operatorname{Re}(\mu) \geq 0$ and $\operatorname{Re}(\mu) = 0$ if and only if $\mu = 0$.

PROOF. From the eigenvalue equation $(A+B)\mathbf{v} = \mu D\mathbf{v}$ we have that

$$(\mathbf{x}, A\mathbf{x}) = \operatorname{Re}(\mu)(\mathbf{x}, D\mathbf{x}) - \operatorname{Im}(\mu)(\mathbf{x}, D\mathbf{y})$$
$$(\mathbf{y}, A\mathbf{y}) = \operatorname{Im}(\mu)(\mathbf{y}, D\mathbf{x}) + \operatorname{Re}(\mu)(\mathbf{y}, D\mathbf{y})$$

where $\mathbf{x} = \text{Re}(\mathbf{v})$ and $\mathbf{y} = \text{Im}(\mathbf{v})$. Note that $(\mathbf{x}, B\mathbf{x}) = 0$ and $(\mathbf{y}, B\mathbf{y}) = 0$, since $B^T = -B$.

From these equations we obtain that

$$\operatorname{Re}(\mu) = \frac{(\mathbf{x}, A\mathbf{x}) + (\mathbf{y}, A\mathbf{y})}{(\mathbf{x}, D\mathbf{x}) + (\mathbf{y}, D\mathbf{y})}.$$

Thus, $\operatorname{Re}(\mu) \geq 0$. If $\mu = 0$, then $\operatorname{Re}(\mu) = 0$. Assume now $\operatorname{Re}(\mu) = 0$ and $\mathbf{v} \neq 0$. We must have necessarily $(\mathbf{x}, A\mathbf{x}) = 0$ and $(\mathbf{y}, A\mathbf{y}) = 0$; then, from Lemma 1, $\mathbf{x} = \mathbf{y} = \mathbf{e}$. It follows that $0 = \operatorname{Im}(\mu)(\mathbf{x}, D\mathbf{y}) = \operatorname{Im}(\mu)(\mathbf{e}, D\mathbf{e})$; thus, $\operatorname{Im}(\mu) = 0$, and then $\mu = 0$.

LEMMA 3. Assume (2)-(5) and let the matrix A + B have the splitting

(7)
$$A+B=M-N$$
, with $\det M \neq 0$.

Let

$$(8) H = M^{-1}N.$$

Then,

- (i) the vector e, defined in (3), is the unique (up to a scalar multiple) eigenvector of H corresponding to the unit eigenvalue;
- (ii) the unit eigenvalue is a simple eigenvalue of H.

PROOF. Part (i): the matrix H may be written as

(9)
$$H = I - M^{-1}(A + B).$$

Since **e** is the unique, apart from a nonzero scalar multiplier, eigenvector of A + B corresponding to the zero eigenvalue (see, part (i) of Lemma 1), from (9) it follows that **e** is the unique eigenvector corresponding to the unit eigenvalue of H.

Part (ii): since zero is a simple eigenvalue of A + B (see, part (ii) of Lemma 1), from $\det(I - H) = (\det M)^{-1} \det(A + B)$ it follows that the unit eigenvalue is a simple eigenvalue of H.

3 – The iterative method

In literature a widely used method for solving (1) is the Method of Simultaneous Displacements with some form of "preconditioning" to the original system (1). This method can be written in the form

(10)
$$\mathbf{u}_{k+1} = \mathbf{u}_k - \tau M^{-1} ((A+B)\mathbf{u}_k - \mathbf{f})$$

or, supposing $\tau = 1$,

(11)
$$M\mathbf{u}_{k+1} = N\mathbf{u}_k + \mathbf{f} \quad k = 0, 1, 2, \dots$$

where M and N are given by the splitting (7) of A + B and \mathbf{u}_0 is an initial estimate of a solution of (1).

We can express the matrix A + B as the matrix sum

$$(12) A+B=D-L-U$$

where $D = \text{diag}\{a_{11}, a_{22}, \ldots, a_{nn}\}$ and L and U are respectively strictly lower and upper triangular $n \times n$ matrices, whose entries are the negative of the entries of A + B respectively below and above the main diagonal of A + B. With this decomposition of A + B an interesting choice of the preconditioner to A + B is the matrix [2]:

(13)
$$M^{-1} = a(\frac{1}{\omega}D - L)^{-1} + (1 - a)(\frac{1}{\omega}D - U)^{-1}$$

where a and ω are real parameters such that $0 \le a \le 1$ and $0 < \omega \le 1$.

In this case the iterative method (11) is characterized by having within its overall mathematical structure certain well-defined substructures that can be executed simultaneously during each iteration k. This feature makes the method (11)-(13) ideally suited for implementation on a parallel vector computer.

The convergence of such a method is guaranteed if and only if the eigenvalues λ_i of the iteration matrix H must satisfy the following two conditions [2]:

(i) $|\lambda_i| \leq 1$ for i = 1, 2, ..., n; $|\lambda_i| = 1$ implies $\lambda_i = 1$;

(ii) all the elementary divisors that correspond to $\lambda_i = 1$ are linear.

From Lemma 3, the elementary divisor that corresponds to the unit eigenvalue of H is linear; thus, in our case, the condition (ii) is satisfied. For condition (i) we have the following result.

THEOREM. Assume (2)-(6) and let the matrix A + B have the splitting (12). Let the matrix M, in the splitting (7), be defined by formula (13). Let $H = H(a, \omega)$ be defined as in (8) where M is given by (13). Then, we have that $\rho(H(a, \omega)) = 1$ and that any complex eigenvalue of H has a modulus less than 1, for ω in a sufficiently small neighborhood of zero; here, $\rho(H)$ is the spectral radius of H.

PROOF. Since $(1, \mathbf{e})$ is an eigen-pair of $H(a, \omega)$ (see, Lemma 3), we have that $\rho(H(a, \omega)) \geq 1$. Note that $\mathbf{e} = (1, 1, \dots, 1)^T$. The matrix M^{-1} , written as

$$M^{-1} = (a(I - \omega D^{-1}L)^{-1} + (1 - a)(I - \omega D^{-1}U)^{-1})\omega D^{-1},$$

may be expressed in the form

$$M^{-1} = a(I + \omega D^{-1}L + \omega^2 (D^{-1}L)^2 + \dots)\omega D^{-1} + (1 - a)(I + \omega D^{-1}U + \omega^2 (D^{-1}U)^2 + \dots)\omega D^{-1}.$$

Thus, for $0 \le \omega \ll 1$, we obtain the following approximation for $H(a, \omega)$:

$$H(a,\omega) = H(a,0) + \frac{\partial H(a,\omega)}{\partial \omega}\Big|_{\omega=0} \omega = I - \omega D^{-1}(A+B)$$

which is independent of a. The eigenvalue equation $H(a, \omega)\mathbf{w} = \lambda \mathbf{w}$ gives

$$\lambda = g(\mu, \omega) = 1 - \mu\omega$$

where μ is an eigenvalue of $D^{-1}(A+B)$.

From Lemma 2 we have that $Re(\mu) > 0$ when $\mu \neq 0$; we have $Re(\mu) = 0$ if and only if $\mu = 0$, which gives $g(0, \omega) = 1$. Thus, from

$$|g(\mu,\omega)|^2 = 1 - 2\text{Re}(\mu)\omega + |\mu|^2\omega^2$$

it follows that

$$\frac{\partial |g(\mu,\omega)|^2}{\partial \omega}\Big|_{\omega=0} = -2\mathrm{Re}(\mu) < 0$$

for $\mu \neq 0$. Therefore, since $g(\mu, 0) = 1$ and 1 is an eigenvalue of $H(a, \omega)$, we have that $\rho(H(a, \omega)) = 1$ and that any complex eigenvalue of H has a modulus less than 1, for ω in a sufficiently small neighborhood of zero.

Thus, for ω in a sufficiently small neighborhood of zero $(0 \le \omega \ll 1)$, the method (11)-(13) converges and

(14)
$$\lim_{k \to \infty} \mathbf{u}_k = \mathbf{u}^*$$

where \mathbf{u}^* is a solution of (1).

With a = 1, method (11)-(13) becomes the SOR method and with $a = \frac{1}{2}$ (11)-(13) becomes the Arithmetic Mean method.

4 – Numerical Experiments

In order to illustrate the sensitivity of the convergence rate to an accurate value of ω and the effectiveness of the method (11)-(13) in obtaining an adequate approximation, some computational experiments have been performed on a test-problem generated by the following difference equation:

(15)
$$-(\alpha u_x + \beta u_y)_{\bar{x}} - (\alpha u_y + \beta u_x)_{\bar{y}} = f(x,y)$$

for all mesh-points (x, y) interior to a rectangular network Ω_h . Here, we have introduced in each mesh-point (x, y) the notation

$$v_{x} = \frac{v(x+h,y) - v(x,y)}{h} \qquad v_{\bar{x}} = \frac{v(x,y) - v(x-h,y)}{h}$$
$$v_{y} = \frac{v(x,y+h) - v(x,y)}{h} \qquad v_{\bar{y}} = \frac{v(x,y) - v(x,y-h)}{h}$$

On the boundary Γ_h of Ω_h the difference equations (15) have been adjusted in such a way that the matrices A and B related to (15) satisfy the conditions (2)-(5).

The matrix A has at most five nonzero elements per row and B has at most seven nonzero entries per row. The order of A and B is n = 4096.

Some results of numerical experiments appear in the Table; k^* is the number of iterations for a maximum-norm of the residual $\mathbf{f} - (A+B)\mathbf{u}_{k^*} = r_{k^*}$ and ω is the relaxation parameter in the matrix M of formula (13). We assume a = 1/2. (The notation 3.7(-02), for instance, means $3.7 \cdot 10^{-2}$).

The initial guess \mathbf{u}_0 of the iterative method (11)-(13) is the null vector.

When we consider the coefficients in (15) $\alpha = \beta = 1$ the triangular matrix L in (12) is a non negative matrix. Similar results are obtained when we consider the coefficients $\alpha = 1$ and $\beta = -1$; in this case the triangular matrix U in (12) is a non negative matrix. With the choice $\alpha = 1$ and $\beta = 2$ in (12) the nonzero entries of L and U are either positive or negative. For $\omega = 1.05$, $\alpha = \beta = 1$ and $\omega = 0.7$, $\alpha = 1$, $\beta = 2$, the iterative method (11)-(13) diverges.

In these experiments a seven-digit accuracy for the approximate solution of (1) has been obtained, using the CRAY Y-MP vector computer.

Let Ω be a bounded, open and connected set of \mathbb{R}^2 with bundary Γ , assumed sufficiently smooth. We consider the boundary value problem

(16)
$$-\operatorname{div}(P \operatorname{grad} u) = \operatorname{div} \mathbf{s} \quad \text{in } \Omega,$$
$$-P \operatorname{grad} u \times \mathbf{n} = \mathbf{s} \times \mathbf{n} \quad \text{on } \Gamma,$$

where P is the matrix

$$P = \begin{pmatrix} p & q \\ -q & p \end{pmatrix}$$

with p > 0, q and $\mathbf{s} = (s_1, s_2)^T$ sufficiently smooth functions in $\overline{\Omega}$. In the boundary condition \mathbf{n} is the outward normal unit vector to Γ ; $\overline{\Omega}$ is the closure of Ω .

Problem (16) is singular, but the solvability condition is satisfied:

$$\int_{\Omega} \operatorname{div} \mathbf{s} \ d\Omega - \int_{\Gamma} \mathbf{s} \times \mathbf{n} \ d\Gamma = 0.$$

The elliptic operator $-\operatorname{div}(P \operatorname{grad} u)$ can be expressed in the equivalent form

 $-\operatorname{div}(P \operatorname{grad} u) = -\operatorname{div}(p \operatorname{grad} u) + \operatorname{div}(u \operatorname{K} \operatorname{grad} q)$

where K is the skew-symmetric matrix

$$K = \begin{pmatrix} 0 & 1\\ -1 & 0 \end{pmatrix}$$

Some basic properties of problem (16) are:

- the adjoint problem of (16) is obtained by replacing P by the transpose matrix P^T in (16);
- let us consider the eigenvalue problem

$$-\operatorname{div}(P \operatorname{grad} u) = \nu \ u \quad \text{in } \Omega,$$

-P grad $u \times \mathbf{n} = 0 \quad \text{on } \Gamma;$

then, $\operatorname{Re}(\nu) \geq 0$ and $\operatorname{Re}(\nu) = 0$ if and only if $\nu = 0$ (to the zero eigenvalue corresponds the solution $u = \text{constant in } \overline{\Omega}$);

1 et c be a positive constant: then, the solution of the problem

$$-\operatorname{div}(P \operatorname{grad} u) + c u = f \ge 0 \quad \text{in } \Omega,$$

$$-P \operatorname{grad} u \times \mathbf{n} = 0 \qquad \text{on } \Gamma,$$

is positive in Ω (maximum principle property).

A suitable finite difference approximation of the continuous problem (16) must produce a matrix equation satisfying the basic properties of the continuous problem outlined above. In paper [1] such a question has been completely analysed: the discrete matrix equation is written in the form (1). In this equation, the matrix A (symmetric and positive semidefinite)

represents the discrete analog to the diffusion operator $-\operatorname{div}(p \operatorname{grad} u)$, together with the boundary condition $-p \operatorname{grad} u \times \mathbf{n} = 0$ on Γ , by means of the usual five-point formulas. The matrix B (skew-symmetric) represents the contribution of the convection operator $\operatorname{div}(u \operatorname{K} \operatorname{grad} q)$.

When in problem (16) we put $p = h_0 \varepsilon / (\varepsilon^2 + f_1^2)$, $q = h_0 f_1 / (\varepsilon^2 + f_1^2)$, $u = g\eta$, $h_0 \mathbf{s} = -P\boldsymbol{\tau}$, where η is the surface elevation, h_0 is the bottom depth, g is the intensity of gravity, $\boldsymbol{\tau}$ is the wind stress, ε is a friction factor and $f_1 = f_0 + \beta y$ is the Coriolins parameter, we obtain the Stommel's model of ocean circulation [7].

We have performed some computational experiments for solving the Stommel's model on a square region of side $L = 2 \cdot 10^6$ m with mesh spacings of the grid $\Delta x = \Delta y = 4 \cdot 10^4$ m. With the parameters $h_0 = 200$ m, $\varepsilon = 10^{-6} \sec^{-1}$, $\boldsymbol{\tau} = (-\cos(\pi y/L), 0)^T$, $f_0 = 2.5 \cdot 10^{-5} \sec^{-1}$ and $\beta = 0$ or $f_0 = 0.5 \cdot 10^{-5} \sec^{-1}$ and $\beta = 10^{-13}$ cm⁻¹ sec⁻¹, the iterative method (11)-(13), a = 1, converges to a solution of (1) for values of the relaxation factor ω of the order of 0.1; some thousands of iterations are needed to have a maximum-norm of the residual $\mathbf{r}_{k^*} = \mathbf{f} - (A + B)\mathbf{u}_{k^*}$ less than 10^{-5} . The initial guess \mathbf{u}_0 is the state of rest.

In all cases the results show exactly the qualitative features of the surface elevation and velocity fields as those reported in [7]. When $f_0 = 0$ and $\beta = 0$, the Gauss-Sidel method, a = 1 and $\omega = 1$, is convergent to a solution of (1) with few hundred of iterations.

$\alpha = \beta = 1$		$\alpha=1,\beta=2$			
ω	k^*	$\ \mathbf{r}_{k^*}\ _\infty$	ω	k^*	$\ \mathbf{r}_{k^*}\ _\infty$
0.1	500	3.7(-02)	0.1	500	3.8(-02)
0.5	430	9.5(-07)	0.3	500	3.0(-05)
0.7	265	9.7(-07)	0.4	482	9.5(-06)
0.9	170	9.5(-07)	0.5	340	1.1(-06)
1.0	130	9.5(-07)	0.6	255	1.0(-06)

Table

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