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NUMERICAL SOLUTION OF EQUILIBRIUM EQUATIONS

HO-JONG JANG

ABSTRACT. We consider some numerical solution methods for equilibrium equations $Af + E^T\lambda = r$, $Ef = s$. Algebraic problems of this form evolve from many applications such as structural optimization, fluid flow, and circuits. An important approach, called the force method, to the solution to such problems involves dimension reduction nullspace computation for E. The purpose of this paper is to investigate the substructuring method for the solution step of the force method in the context of the incompressible fluid flow. We also suggests some iterative methods based upon substructuring scheme.

1. Introduction

Equations of equilibrium arise in numerous areas of science and engineering. Applications to structures, fluid flow, electric networks, and signal processing are elegantly described in Strang [8]. An **equilibrium matrix** (or **incidence matrix**) is an $m \times n$ matrix E generally associated with a finite difference or finite element grid, a graph or a network. When the problem is modeled using domain decomposition or substructuring techniques, E is highly structured.

The context in which equilibrium matrices arise may be stated as the quadratic programming problem: minimize $f^TAf - 2f^Tr$ subject to $Ef = s$, and first-order necessary conditions for a solution to this problem are

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given by the system of linear equations

$$\begin{bmatrix} A & E^T \\ E & 0 \end{bmatrix} \begin{bmatrix} f \\ \lambda \end{bmatrix} = \begin{bmatrix} r \\ s \end{bmatrix}, \tag{1}$$

where λ is a vector of Lagrange multiplier.

The fluid flow problems are formulated in terms of the Navier-Stokes equations, and when appropriately discretized, give rise to the Lagrange multipliers problem(1) (see [3]). The vector f represents velocity, while λ is pressure. The equilibrium matrix E is a discrete divergence operator, while A is the $n \times n$ discretization of convective and diffusion effects. A has block tri-diagonal structure, but is generally not symmetric. The equations $Ef = s$ and $Af + E^T\lambda = r$ reflect conservation of mass and conservation of momentum, respectively; the vector r and s capture boundary and forcing terms.

In the force method (or dual variable method), the vector f is computed in three phases:

i) Solve $Ef_p = s$, f_p is any particular solution to $Ef = s$, and find a nullspace N of E.

ii) Let the columns of N be the null basis of E, and solve

$$N^TANf_0 = -N^T(r - Af_p). \tag{2}$$

iii) Set $f = f_p + Nf_0$, and solve $E^TE\lambda = -EAf$.

The force method is a dimension reduction scheme based upon computation of a basis for the nullspace for E. Nullspace computation of the force method has an important role in the entire force method computation.

In our approach to compute the nullspace we use a parallel scheme by utilizing the graph theoretic ideas in what we call the **substructuring method**, which is introduced by Plemmons and White[7]. This method successfully handles parallel nullspace computation, and several implementation details are reported in [4]. Here we continue the study of the substructuring method for the solution step of the force method, which is system (2).

With discussion about the solvability of system (2), development of a iterative scheme based on the substructuring method and comparison with some other methods in terms of numerical efficiency and parallel computation aspects are our main purposes of this paper.

2. Substructuring method

In general, there exists a product of elementary matrices, P, such that

$$PE = [E_1, E_2] = E_1[I_m, E_1^{-1}E_2],$$

where E_1 is nonsingular. Consequently, the nullspace of PE, and hence E, is generated by the columns of the block matrix

$$N = \begin{bmatrix} E_1^{-1}E_2 \\ -I_{n-m} \end{bmatrix}.$$

Methods of finding a sparse or structural basis of the nullspace of the equilibrium matrix have been the subjects of extensive study over the past few years. With special interest in parallel computation, motivation for developing the substructuring method was that the nullspace computation(forming N) can often be done by appropriate ordering of the nodes and elements, extending certain results in [2]. This ordering yields a matrix E with a great deal of structure which can be exploited by multiprocessing computers in forming N.

We consider an application of the substructuring method, the proper partition of the finite difference grid, to the incompressible Navier-Stokes equations. The matrix A will change a little from one time step to next. With an appropriate ordering cf the nodes and elements, a matrix E, which reflects the conservation of mass equation, has a block angular form in the most of the fluid flow case [7]. The resulting nullspace basis matrix N normally has the form:

$$N = \begin{bmatrix} n_{11} & & & & \\ n_{21} & n_{22} & & & \\ & n_{32} & \ddots & & \\ & & \ddots & n_{tt} & \\ & & & n_{t+1,t} & \\ & & -I & & \end{bmatrix}, \tag{3}$$

where n_{ij} is upper triangular matrix which has components are 1 for $i = j$, and are -1 for $i \neq j$. Here, $\dim(n_{ij})$ is the number of elements for each structure, and t is the number of sets in the partition of the nodes.

More details of the nullspace computation based upon the substructuring method are in [7].

3. System (2) with substructuring method

In this section we discuss the solvability of (2) and consider iterative methods in parallel and substructuring aspects.

3.1. Solvability of system (2)

The following results from Amit et al. [1] and Hall [3] do establish sufficient conditions for the nonsingularity of N^TAN.

THEOREM 3.1. *If $Y^TAY \neq 0$ for all non-zero Y in the range $\mathcal{R}(N)$ of the matrix N, then N^TAN is nonsingular.*

THEOREM 3.2. *If*
(i) *A has positive diagonal elements,*
(ii) *A is both row and column diagonally dominant, and A is strictly diagonally dominant in the either rows or columns, and*
(iii) *N has full row rank,*
then N^TAN is nonsingular.

In fact, in the incompressible fluid flow with uniform mesh spacing case, the diagonal dominance of A is a natural condition. The difficult hypothesis to satisfy is the diagonal dominance of A^T. One way to guarantee this is to restrict the time step. From the properties of A in incompressible fluid flow case, we established more results in [5].

The next results show that the block banded shape of N^TAN based on the substructuring method.

THEOREM 3.3. *Let N be the nullspace of the incidence matrix, which has the form in (3). Then the matrix $P = N^TAN$ has the following properties:*
(i) *Suppose* $A = \begin{bmatrix} A_x & 0 \\ 0 & A_y \end{bmatrix}$ *and* $N = \begin{bmatrix} N_1 \\ -I \end{bmatrix}$. *Then P can be expressed as $N_1^TA_xN_1 + A_y$, where A_x, A_y: discretization of momentum equation for x, y direction, respectively.*
(ii) *P is block-pentadiagonal.*
(iii) *The size of each block of P depends on the number of elements in each partition of substructures.*

PROOF. (i)

$$P = [N_1^T, -I] \begin{bmatrix} A_x & 0 \\ 0 & A_y \end{bmatrix} \begin{bmatrix} N_1 \\ -I \end{bmatrix} = N_1^T A_x N_1 + A_y.$$

(ii) Suppose N has the form as in (3). Then

$$N_1^T A_x N_1 = \begin{bmatrix} n_{11}^T(a_{11}n_{11} + a_{12}n_{21}) & n_{11}^T a_{12} n_{22} & n_{21}^T a_{23} n_{33} & & \\ +n_{21}^T(a_{21}n_{11} + a_{22}n_{21}) & +n_{21}^T(a_{22}n_{22} + a_{23}n_{32}) & & & \\ n_{22}^T(a_{21}n_{11} + a_{22}n_{21}) & \ddots & \ddots & \ddots & 0 \\ +n_{32}^T a_{23} n_{21} & & & & \\ n_{33}^T a_{32} n_{21} & \ddots & & & \\ 0 & \ddots & & & \end{bmatrix}.$$

Note that $\dim(n_{ij})=\dim(a_{ij})$, and each a_{ii} is a triangular matrix with positive diagonal entries and off-diagonal entries are negative, and a_{ij} is diagonal matrix with negative entries if $i \neq j$. Since A_y is block tridiagonal matrix, $P = N_1^T A_x N_1 + A_y$ is a block pentadiagonal matrix.

(iii) By (ii), it is obvious. □

3.2. Iterative methods

Recall that $N^T AN$ is not an M-matrix and is also nonsymmetric. Although any iterative method can be formally applied to this nonsymmetric problem, in most cases there is no guarantee that the iterative method will converge. Many iterative methods were proposed and discussed in [6] to solve (2). In addition to these, we proposed a iterative method which can take advantage of using the substructuring method. We now pick the best among the other iterative methods which were suggested in [6] and consider its parallel and substructuring aspects.

Induced Jacobi method (IJ). This method [6] comes from splitting the matrix A into $A_d - A_l - A_u$ and then gets the product form:

$$N^T AN = N^T(A_d - A_l - A_u)N,$$

where A_d is a diagonal matrix which has only diagonal part of A and $A_l + A_u = A_d - A$. Now, just as with the standard Jacobi method, we get

$$\begin{aligned} N^T A_d N f_0^{k+1} &= N^T(A_l + A_u)N f_0^k + b, \\ \text{and} \quad f_0^{k+1} &= M_J f_0^k + (N^T A_d N)^{-1} b, \end{aligned} \tag{4}$$

where $b = -N^T(r - Af_p)$, $M_J = (N^T A_d N)^{-1}(N^T(A_l + A_u)N)$. Since A_d is a diagonal matrix with positive components, which satisfies the hypothesis of the Theorem 3.2, $N^T A_d N$ is invertible.

Block Induced Jacobi method (BIJ). Recall that A is block tridiagonal matrix and N also has block structure based on the substructuring method. By using these facts, this iterative method can be obtained in the same way as the induced Jacobi method except we take A_D for the splitting matrix. We have

$$\begin{aligned} N^T A_D N f_0^{k+1} &= N^T(A_L + A_U)N f_0^k + b, \\ \text{and} \quad f_0^{k+1} &= M_B f_0^k + (N^T A_D N)^{-1} b, \end{aligned} \tag{5}$$

where $M_B = (N^T A_D N)^{-1}(N^T(A_L + A_U)N)$, A_D is a block diagonal matrix with components from only block diagonal part of A and $A_L + A_U = A_D - A$. Here, A_D also satisfies the hypothesis of the Theorem 3.2, and $N^T A_D N$ is invertible.

It is difficult to say that (4) and (5) are always convergent without any restriction because properties of the matrix A depend on time step, mesh lengths and density etc. One way to prove that (4) and (5) are convergent is to find suitable conditions under which the modulus of the eigenvalues of M_J and M_B are less than one. We will need the following definition.

DEFINITION. A square matrix, F is
Hermitian Positive Definite (*HPD*) iff $\mathrm{Re}(x^T(F + F^T)x) > 0$ for all $x \neq 0$ and F is Hermitian,
Complex Positive Definite (*CPD*) iff $\mathrm{Re}(x^H(F + F^T)x) > 0$ for all $x \neq 0$ and F is Complex.

LEMMA 3.4. *If F is a Hermitian $n \times n$ strictly diagonally dominant or irreducibly diagonally dominant matrix with positive real diagonal entries, then F is HPD.*

PROOF. See Varga [9] □

LEMMA 3.5. *If A is CPD and N has full column rank, then N^TAN is also CPD and hence nonsingular.*

PROOF. Let $x \in \mathcal{C}^{n-m}/\{0\}$ and define $z = Nx$. Then $z \neq 0$, because N has full column rank. So $Re(x^H(N^TAN+(N^TAN)^T)x) = Re(x^H(N^TAN+(N^TA^TN)x) = Re(x^HN^T(A+A^T)Nx) = Re(z^H(A+A^T)z) > 0$, because A is CPD. And since $Re(x^H(N^TAN)x) = Re(\frac{1}{2}x^H(N^TAN+(N^TAN)^T)x) > 0$, N^TAN is nonsingular. □

THEOREM 3.6. *If A and A^T are diagonally dominant and either A or A^T is strictly diagonally dominant, then (4) and (5) are convergent.*

PROOF. We only show that the convergence of BIJ, (5). The proof of the convergence of IJ is in [6]. Let λ be an eigenvalue of M_B in (5), and let x be an eigenvector associated with λ. Then

$$
\begin{aligned}
M_Bx = \lambda x \quad &\Rightarrow \quad (N^TA_DN)^{-1}[N^T(A_L + A_U)N]x = \lambda x \\
&\Rightarrow \quad \frac{1}{\lambda}[N^T(A_L + A_U)N]x = N^TA_DNx \qquad (6) \\
&\Rightarrow \quad [N^T(\frac{1}{\lambda})(A_L + A_U)N]x = N^TA_DNx \\
&\Rightarrow \quad N^T[A_D - \frac{1}{\lambda}(A_L + A_U)]Nx = 0.
\end{aligned}
$$

Define the matrix-valued function $C(\lambda) \equiv A_D - \frac{1}{\lambda}(A_L + A_U)$. Let $|\lambda| \geq 1$. Without loss of generality, assume A is strict row diagonally dominant. Then, we have

$$
\begin{aligned}
&|a_{kk}| > \sum_{j\neq k} |a_{kj}| = |a_{k,k+1}| + |a_{k,k-1}| + \sum_{j\neq k-1,k,k+1} |a_{kj}| \\
\Rightarrow \quad &|a_{kk}| - [|a_{k,k+1}| + |a_{k,k-1}|] > \sum_{j\neq k-1,k,k+1} |a_{kj}|,
\end{aligned}
$$

where a_{ij} is component of A. Since off-diagonal entries of A are negative, $|a_{k,k-1}| + |a_{k,k+1}|$ is the same as $|a_{k,k-1} + a_{k,k+1}|$, and

$$|a_{kk} - (a_{k,k+1} + a_{k,k-1})| \geq |a_{kk}| - |a_{k,k+1} + a_{k,k-1}|.$$

Hence,

$$|a_{kk} - (a_{k,k+1} + a_{k,k-1})| > \sum_{j\neq k-1,k,k+1} |a_{kj}| \geq \frac{1}{|\lambda|} \sum_{j\neq k-1,k,k+1} |a_{kj}|.$$

Note that above inequality also holds for the case that either $a_{k,k+1}$ or $a_{k,k-1}$ is zero. By using the diagonal dominance of A^T and from the same argument as above, we have

$$|a_{kk} - (a_{k+1,k} + a_{k-1,k})| \geq \frac{1}{|\overline{\lambda}|} \sum_{j \neq k-1,k,k+1} |a_{jk}|.$$

Adding two previous inequalities, we obtain

$$\begin{aligned} &|2a_{kk} - (a_{k,k+1} + a_{k,k-1} + a_{k+1,k} + a_{k-1,k})| \\ &> \frac{1}{|\lambda|} \sum_{j \neq k-1,k,k+1} |a_{kj}| + \frac{1}{|\overline{\lambda}|} \sum_{j \neq k-1,k,k+1} |a_{jk}| = \sum_{j \neq k-1,k,k+1} (|\frac{a_{kj}}{\lambda}| + |\frac{a_{jk}}{\overline{\lambda}}|) \\ &\geq \sum_{j \neq k-1,k,k+1} |\frac{a_{kj}}{\lambda} + \frac{a_{jk}}{\overline{\lambda}}|. \end{aligned}$$

Since A_D is block diagonal and each block has 3 non-zero diagonals which are a_{kk}, $a_{k+1,k}$, and $a_{k-1,k}$, the matrix $C(\lambda) + C(\lambda)^H$ is strictly diagonally dominant, Hermitian and has positive diagonal entries. Hence, it is HPD by Lemma 3.4, and $C(\lambda)$ is CPD and therefore invertible. Now from Lemma 3.5, $N^T C(\lambda) N$ is CPD and thus invertible also. That means that if $|\lambda| \geq 1$, then there can be no non-zero vector, x, such that $N^T C(\lambda) N x = 0$, which contradicts (6). This contradiction implies that $|\lambda| < 1$, and BIJ is convergent. □

Restrictions on mesh-spacing and time-step are the requirements for the diagonally dominance of A and A^T. We need to require the condition about time-step for the diagonally dominance of A^T, because A is strictly diagonally dominant when mesh-spacing are constant in the incompressible fluid flow case. More results related to restrictions on time-step and the inner computation of (2) are discussed in [5].

4. Numerical experiments

We consider the implementation of the BIJ and discuss some numerical results comparing the performance of IJ and BIJ. The problem chosen was the 2D driven cavity problem that is well known as a standard test problem in fluid mechanics. The fluid contained in a square cavity is subjected to a uniform velocity imposed upon the top surface. We set the viscosity μ=0.025, which is equivalent to the case of a Reynolds' number

of 400. The region was overlaid with 8×8 grids of uniform mesh which means the dimension of A matrix is 136×136. Uniform time step of 1 second was chosen and the inner and outer convergence tolerance was set at 10^{-5}. Calculations were done on an Alliant FX/40 with two vector CPU's.

We display in Table 1 the comparison of BIJ and IJ for outer loop, and inner computations were done by either block SOR or point SOR. From Table 1 we see that BIJ for the outer loop and the block SOR for the inner loop was best among those tested. According to Table 2, we get the best speedup when we use IJ for outer loop and point SOR for inner loop in parallel computation.

TABLE 1. The matrix A of order n=136; Inner Optimal ω= 1.84

Outer	BIJ							
Inner	block SOR				point SOR			
Time step	1	2	3	4	1	2	3	4
Outer iter.	25	20	27	18	25	22	18	18
CPU Time(sec.)	1.325	1.309	0.891	0.674	2.345	2.711	1.510	1.144

Outer	IJ							
Inner	block SOR				point SOR			
Time step	1	2	3	4	1	2	3	4
Outer iter.	38	27	43	20	38	32	31	20
CPU Time(sec.)	3.750	2.716	2.026	1.508	3.739	2.735	1.951	1.426

TABLE 2. Summary of speedups for each iterative method
(after 5 time steps)
($-O_g$: optimized serial; $-O$: concurrent with vectorization)

Outer	Inner	$-O_g$		$-O$		Speedup
BIJ	block SOR	15	2.064	15	0.552	3.74
	point SOR	15	5.101	15	0.802	6.36
IJ	block SOR	17	3.982	17	1.008	3.95
	point SOR	18	6.771	18	0.950	7.13
		iter.	time	iter.	time	

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Department of Mathematics
Hanyang University
Seoul 133-791, Korea
E-mail: hjang@fermat.hanyang.ac.kr