SPARSE MATRIX METHOD FOR EQUILIBRIUM EQUATION

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Abstract. We consider some numerical solution method for the 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 structural analysis and fluid flow. In structural analysis we adopt linearly constrained sum-of-squares schemes to the solution step of the force method and examine this scheme based on substructuring method. A number of interesting characterizations of this problem are discussed, and some parallel iterative schemes are suggested. These schemes are based upon transformed iterative methods and substructuring concepts.

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 [14]. 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. Upon aggregation and then scaling, E can often be assumed to have entries 0 and ± 1. When the problem is modeled using domain decomposition or substructuring techniques, E is also highly structured.

The context in which equilibrium matrices arise may be stated in two forms:

Constrained Minimization Problem

$$\text{Minimize } f^TAf - 2f^Tr \quad \text{subject to} \quad Ef = s, \tag{1}$$

Lagrange Multiplier Problem

$$\begin{bmatrix} A & E^T \\ E & 0 \end{bmatrix} \begin{bmatrix} f \\ \lambda \end{bmatrix} = \begin{bmatrix} r \\ s \end{bmatrix}. \tag{2}$$

The matrix A is generally some symmetric nonnegative definite matrix associated with the minimization problem. For example, A is the element flexibility matrix in the context of structural analysis.

The structures problem of computing the system forces, displacements and associated stresses and strains is usually formulated as minimization of potential energy of the elements in the structure, leading to a constrained minimization problem of the form (1). In this case $r = 0$, s is the vector of external loads, f is the system force vector and $-\lambda$ is the displacement vector associated with (2). Here A is symmetric and block diagonal, where each block is associated with an element of the structure and has relatively small dimension. In this case Lagrange formulation can be viewed as least squares problem with equality constraints(LSE):

$$\text{Minimize } \|Gf - c\|_2 \quad \text{subject to} \quad Ef = s. \tag{3}$$

Here G and c in LSE are related to A and r in the other formulations by $r = G^Tc$ and $A = G^TG$.

The fluid flow problems are formulated in terms of the Navier-Stokes equations, and when appropriately discretized, give rise to the Lagrange multipliers problem(2) (see [5]). 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. If we restrict our discussion of fluid flows applications to Stokes(non-convective) flow, in which the matrix A is in fact symmetric positive definite, formulation (1) also can be viewed as (3). Several methods for solving problems of the form of (3) are described in [3].

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There are two methods generally used to calculate the solution of (1) or (2), the displacement method and the force method. The relative merits of the two approaches have been the topic of some debate [5, 9]. In this paper we deal with the force method.

Force Method. Consider (2) and under the reasonable conditions, so that N^TAN is invertible where N is a matrix whose columns form a basis of the nullspace of E.

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

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

$$N^TANf_0 = -N^T(r - Af_p). \tag{4}$$

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

A force method may be preferable when 1) N is readily computable and, 2) dimensions m, n are such that $n - m \ll m$. Then since N^TAN has order $n - m$ while $EA^{-1}E^T$ has order m, 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 computing 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 [13]. This method successfully handles parallel nullspace computation. The focus of this paper is the use of both the substructuring and the force method, henceforth refered to as **SFM**, for the structural analysis and incompressible fluid flow problems.

2. Substructuring Method. In general, there exists a product of elementary matrices, P, such that

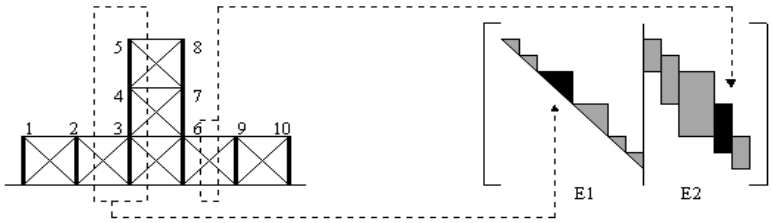
$$PE = [E_1, E_2] = E_1[I_m, E_1^{-1}E_2],$$

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 has been the subject of extensive study over the past few years(see, for example [2, 6]). 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, 4]. This ordering yields a matrix E with a great deal of structure which can be exploited by multiprocessing computers in forming N. Substructuring with proper partition of the flexible truss, for example, leads to matrix E resembling that depicted in Figure 1. The blocks in E are usually sparse(see Plemmons and White [13] for details).

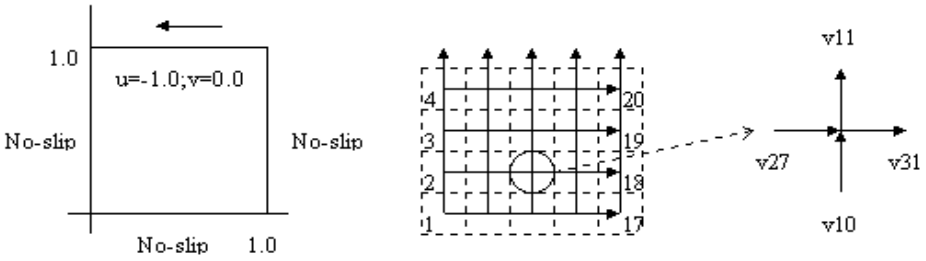
FIG. 1. *6 Disjoint substructures and its equilibrium matrix*



We consider an application of the substructuring method, the proper partition of the finite difference grid, to the incompressible fluid flow. As mentioned in §1, an appropriate discretization of the Navier-Stokes equations will yield a sequence of problems of the form (2). The matrix A will change a little from one time step to next in fluid case. As E reflects the conservation of mass equation, it remains fixed.

The driven cavity problem is presented in which the substructuring method with proper partition has been successfully applied on practical fluid flow problem.

FIG. 2. *Driven cavity with finite difference grid*



A finite difference grid with 20 cells has 36 unknown velocity components is illustrated in Figure 2. Each cell is analogous to a free node and each vector component is analogous to an element. The nodes at the top of vectors v_4, v_8, v_{12}, v_{16} and v_{20} are fixed nodes. The connected graph is now directed and the corresponding equilibrium matrix has entries 0 and ± 1, and is called an incidence matrix in Hall [5]. The associated equilibrium matrix E has the following form:

$$\left[\begin{array}{cccc|ccccc} f & & & & i & & & & \\ & f & & & -i & i & & & \\ & & f & & & -i & i & & \\ & & & f & & & -i & i & \\ & & & & f & & & & -i \end{array}\right], \; f = \left[\begin{array}{cccc} 1 & & & \\ -1 & 1 & & \\ & -1 & 1 & \\ & & -1 & 1 \end{array}\right], \; i = \left[\begin{array}{cccc} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{array}\right].$$

For example, row 11 in the incidence matrix reflects the conservation of mass for cell 11:

$$\frac{v_{31} - v_{27}}{h} + \frac{v_{11} - v_{10}}{h} = 0, \text{ where } h = \Delta x = \Delta y.$$

The resulting nullspace basis matrix N has the form:

$$N = \left[\begin{array}{cccc} f^{-1} & & & \\ -f^{-1} & f^{-1} & & \\ & -f^{-1} & f^{-1} & \\ & & -f^{-1} & f^{-1} \\ & & & -f^{-1} \\ & & \text{-I} & \end{array}\right], \; f^{-1} = \left[\begin{array}{cccc} 1 & & & \\ 1 & 1 & & \\ 1 & 1 & 1 & \\ 1 & 1 & 1 & 1 \end{array}\right].$$

More discussion of the nullspace computation about an obstacle case is reported in [8].

3. SFM in Structural Analysis. Given a paticular solution f_p of the equilibrium equation, the main task of SFM in structural analysis is the computation of the redundant force vector f_0 which satisfies system (4). Then the system force vector f is given by $f_p + Nf_0$. System (4) is simply the normal equation for the weighted least squares problem:

$$\text{Min}_{f_0} \|G^{-1}(Nf_0 + f_p)\|_2, \tag{5}$$

where G is Cholesky factor of element stiffness matrix A^{-1}. Several methods for solving problems of the form (5) are described in [3]. However, poor results may be obtained with most of the traditioinal methods when the element flexibility matrix A is ill-conditioned. In a series of papers [11, 12], Paige has developed schemes which can considerably reduce this difficulty. Paige's new schemes for linearly constrained sum-of-squares(LCSS) problem to (5) with trunback QR factorization for nullspace computation are discussed in [6]. Furthermore, these new schemes have been successfully applied to rapid reanalysis of structures, and reported in [7].

Paige's Formulations. Paige[12] has given a formulation of LCSS in which the two orthogonal transformation Q and U are computed simultaneously in a manner which retains the triangular structure of G throughout the computation. The result is a factorization of the form

$$Q^T[f_p, N, GU] = \left[\begin{array}{cccc} f_{p1} & 0 & M_1 & 0 \\ f_{p2} & R^T & M_{21} & M_2 \end{array}\right], \tag{6}$$

where R^T, M_1, and M_2 are lower triangular matrices of order $n-m$, m, and $n-m$, respectively, and Q and U are orthogonal matrices of order n. Applying transformation (6) and using the change of variable $U^T v = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$, where $v = G^{-1}(Nf_0 + f_p)$, problem (5) becomes

$$\text{Min} v_1^T v_1 + v_2^T v_2$$

$$\text{subject to} \quad \begin{bmatrix} M_1 & 0 \\ M_{21} & M_2 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} 0 \\ R^T \end{bmatrix} f_0 + \begin{bmatrix} f_{p1} \\ f_{p2} \end{bmatrix}. \tag{7}$$

The constraints show that v_1 is fully determined since M_1 has full column rank, and we can minimize the functional by taking $v_2 = 0$. Finally the solution f_0 now be determined from the system

$$R^T f_0 = M_{21} v_1 - f_{p2}.$$

Note that in our case, full column rank of N and Cholesky factor G leads to triangular matrices in the factorization (7).

4. SFM in Fluid Flow. SFM for the incompressible fluid flow problem is only useful as a computational tool if the coefficient matrix, $N^T AN$(in (4)), is nonsingular. In general, $N^T AN$ being nonsingular is not guaranteed by the nonsingularity of A itself. In this section we discuss the solvability of (4) and consider iterative methods in parallel and substructuring aspects. In order to consider these problems, we focus on the structures of the coefficient matrix of (4) based on the substructuring method, and we also develope a nested iterative method.

4.1. Solvability of System (4). The following results from Amit et al. [1] and Hall [5] do establish sufficient conditions for the nonsingularity of $N^T AN$.

THEOREM 4.1. *If $Y^T AY \neq 0$ for all non-zero Y in the range $\mathcal{R}(N)$ of the matrix N, then $N^T AN$ is nonsingular.*

THEOREM 4.2. *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 column rank,
then $N^T AN$ 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 [8].

The block banded structure of $N^T AN$ based on the substructuring method gives us much advantages for the entire parallel computation including the inner system computation when we use the iterative methods.

THEOREM 4.3. *Let N be the nullspace of the incidence matrix, then the matrix $P = N^T AN$ 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 $N_1^T A_x N_1 + A_y$, where A_x, A_y: discretization of momentum equation for x, y direction, respectively.
(ii) P is block-pentadiagonal matrix,
(iii) The size of each block of P depends on the number of elements in each partition of substructures,
(iv) If mesh-spacing is constant, and P_{ij} is the ijth block of the matrix P, then the signs of the each block are:

$$\begin{cases} P_{ij} \leq 0 & \text{if } |i-j| = 1 \\ P_{ij} \geq 0 & \text{if } |i-j| = 2 \\ P_{ij} = 0 & \text{otherwise.} \end{cases}$$

4.2. Iterative Methods. We consider the SFM for the incompressible fluid flow problem via iterative methods. Direct techniques have been used to solve (4), see [1].

The time step restriction has an important role for not only the solvability of (4) but the convergence of the iterative methods. Conditions which guarantee the convergence of the some iterative methods to solve (4) for real values of the time step are presented in [10]. However, bound conditions for time step restriction have been exceeded with no ill effects on the convergence of the iterative methods. In [8], enhancement of those conditions and related theorems are presented. In fact, it turns out to be similar to the *Courant number* condition when the mesh-spacing is constant.

Recall that N^TAN 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 [10] to solve (4). In addition to these, we proposed an iterative method which can take advantage of using SFM. We now pick the best among other iterative methods which were suggested in [10] and consider its parallel and substructuring aspects with our iterative method.

Induced Jacobi method(IJ). This method [10] comes from splitting the matrix A into $A_d - A_l - A_u$ and then gets the product form:

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

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

$$N^TA_dNf_0^{k+1} = N^T(A_l + A_u)Nf_0^k + b,$$

and

$$f_0^{k+1} = M_Jf_0^k + (N^TA_dN)^{-1}b, \tag{8}$$

where $b = -N^T(r - Af_p)$, $M_J = (N^TA_dN)^{-1}(N^T(A_l + A_u)N)$. Since A_d is a diagonal matrix with positive components, which satisfies the hypothesis of the Theorem 4.2, N^TA_dN 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

$$N^TA_DNf_0^{k+1} = N^T(A_L + A_U)Nf_0^k + b,$$

and

$$f_0^{k+1} = M_Bf_0^k + (N^TA_DN)^{-1}b, \tag{9}$$

where $M_B = (N^TA_DN)^{-1}(N^T(A_L + A_U)N)$, 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 4.2, and N^TA_DN is invertible.

It is difficult to say that (8) and (9) are always convergent without any restriction because properties of the A matrix depend on time step, mesh lengths and density etc. One way to prove that (8) and (9) 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 1. 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 4.4. *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.*

LEMMA 4.5. *If A is CPD and N has full column rank, then N^TAN is also CPD and hence non-singular.*

THEOREM 4.6. *If A and A^T are diagonally dominant and either A or A^T is strictly diagonally dominant, then (8) and (9) are convergent.*

Restrictions on mesh-spacing and time-step are the requirements for the diagonal dominance of A and A^T. We need to give 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 are discussed in [8].

4.4. Numerical Experiment. 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.

We display in Table 1 the comparison of BIJ and IJ for outer loop, and inner computation 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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