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SPARSE NULLSPACE COMPUTATION OF EQUILIBRIUM MATRICES

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ABSTRACT. We study the computation of sparse null bases of equilibrium matrices in the context of structural optimization and incompressible fluid flow. In our approach we emphasize the *parallel computation* and examine the applications. New block decomposition and node ordering schemes are suggested, and numerical examples are considered.

1. Introduction

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. The matrix E, which typically represents the interconnections among the members of the system being modeled, is usually sparse and of full row rank m. After scaling, E can often be assumed to have entries 0 and ± 1. An excellent general discussion of equilibrium matrices can be found in the work of Strang [13], where applications to structures, fluid flow, electric networks, and signal processing are described in detail. The context in which equilibrium matrices arise is generally stated in two forms:

Constrained Minimization Problem

$$\min\ y^T F y - 2y^T s \quad \text{subject to} \quad Ey = p, \tag{1}$$

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Lagrange Multiplier problem

$$\begin{bmatrix} F & E^T \\ E & 0 \end{bmatrix} \begin{bmatrix} y \\ \lambda \end{bmatrix} = \begin{bmatrix} s \\ p \end{bmatrix}. \tag{2}$$

In this paper we are interested in applications to structural analysis and fluid flow computations. 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 $s = 0$, p is the vector of external loads, y is the system force vector and $-\lambda$ is the displacement vector associated with (2). Here F is symmetric and block diagonal, where each block is associated with an element of the structure and has relatively small dimension.

The fluid flow problems are formulated in terms of the Navier-Stokes equations, and when appropriately discretized, gives rise to the Lagrange multipliers problem (2) (see [8] and [13]) The vector y represents velocity, while λ is pressure. The equilibrium matrix E is a discrete divergence operator, while F is the $n \times n$ discretization of convective and diffusion effects. F has block tri-diagonal structure, but is generally not symmetric. The equations $Ey = p$ and $Fy + E^T\lambda = p$ reflect conservation of mass and conservation of momentum respectively; the vector p and s capture boundary and forcing terms.

There are two methods generally used to calculate (1) or (2), the displacement method and the force method. In this paper we discuss the nullspace computation occurs in the force method. The force method, as derived in [1], is now summarized.

Force Method Consider (2) and assume N^TFN is invertible, where N is a matrix whose columns form a basis of the nullspace of E.

(i) Solve $Ef_p = s$, f_p is any particular solution to $Ef = s$.

(ii) Find a basis of the nullspace N of E, and solve

$$N^TFNf_0 = -N^TFf_p, \ f_0 \text{ is a redundant force vector.}$$

(iii) Set $f = f_p + Nf_0$.

The existence and uniqueness of solution to problems (1) and (2) are generally given by two sets of assumptions leading to well-known theorems. The first theorem is relevant to the structures problem and

the second is important in fluid flow computations. Discussions of the first theorem and the second theorem can be found in Dyn and Ferguson [5] and Hall [8], respectively.

THEOREM 1. *If i) F is symmetric and nonnegative definite, ii) E has full row rank, and iii) F and E have no common null vector, then problems (1) and (2) are equivalent and have a unique solution.*

THEOREM 2. *If i) F has positive diagonal elements, ii) F is both row and column diagonally dominant and is strictly diagonally dominant in the rows or columns, and iii) E has full row rank then the linear system (2) has a unique solution.*

The purpose of this paper is to develop some schemes for computing a basis of the nullspace of an equilibrium matrix. Methods of finding a sparse or structured basis of the nullspace of E has been the subject of extensive study over the past few years [7][14][10][9][2][3.4].

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

$$PE = [R_1, R_2] = R_1[I_m, R_1^{-1}R_2], \tag{3}$$

where R_1 is nonsingular. Consequently, the nullspace of PE, and hence E, is generated by the columns of the block matrix

$$N = \begin{bmatrix} R^{-1}R_2 \\ -I_{n-m} \end{bmatrix}. \tag{4}$$

Even though the null basis is not unique, we are interested in those which are sparse and banded. Nullspace computation(forming N) can often be done by appropriate ordering of the nodes and elements, extending certain results in Berry et al. [2], Gilbert and Heath [6]. This ordering yields a matrix E with a great deal of structure which can be exploited by multiprocessing computers in forming N. This has been a topic of recent interest in the literature; Plemmons and White [11], Stern and Vavasis [12].

2. Nullspace Computation with Substructure Scheme

In this section we will use the parlance of the finite element models for physical structures; For a given undirected graph $\mathcal{G}$ with node set $\mathcal{N}$ and set of edges $\mathcal{E}$, we write $\mathcal{S}=(\mathcal{N},\mathcal{E})$ and say $\mathcal{S}$ a structure if the graph $\mathcal{G}$ is connected. We may think of edges, (i,j), as elements connecting the nodes i and j. A pair $\mathcal{S}_1 = (\mathcal{N}_1, \mathcal{E}_1)$ is a substructure of $\mathcal{S}$ if $\mathcal{N}_1$ and $\mathcal{E}_1$ are nonempty subsets of $\mathcal{N}$ and $\mathcal{E}$, respectively, and $\mathcal{S}_1$ is itself a structure.

DEFINITION 1. Let $\mathcal{S} = (\mathcal{N}, \mathcal{E})$ be a structure, where $\mathcal{N}$ has cardinality m and $\mathcal{E}$ has cardinality n. An *equilibrium matrix of* $\mathcal{S}$ is a $m \times n$ matrix $E=(e_{ij})$, where

$$e_{ij} = \begin{cases} 1 & i \in \mathcal{N} \text{and } j = (i,k) \in \varepsilon \text{ for some } k \in \mathcal{N} \\ 0 & \text{otherwise.} \end{cases}$$

In general, we call a structure with matrix E stable if E has full row rank. A stable structure always has a null basis matrix N which can be expressed in the form (4).

EXAMPLE 1. This is an example of a pin-jointed-truss with 10 nodes and 31 elements. In this case each node has 2 associated forces, and consequently, the matrix E is 20×62.

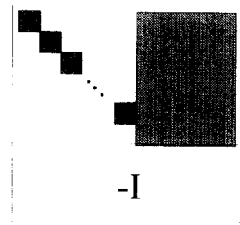
FIGURE 1: Pin-Jointed-Truss and its Equilibrium Matrix

The substructures 1 and 2 in Figure 1 are stable while 3 is not stable. Our main interest here is to find a nullspace basis matrix which can be computed in parallel. For this purpose, if the connecting elements for

each substructure are associated with the last block of nodes, then the equilibrium matrix takes the block angular form in Figure 1. The first 3 blocks for E are associated with substructures.

More details about node/element numbering and the following theorem are described in Plemmons and White [11].

THEOREM 3. *Let $\mathcal{S} = (\mathcal{N}, \mathcal{E})$ be a stable structure with an associated partition. Then with the equilibrium matrix E assembled into the form of Figure 1. there is a basis matrix N of the nullspace of E such that for some permutation matrix P, PN has the following block form:*



From the observation of Example 1, we can assume that a reasonably good scheme is used for substructures and numbering nodes and elements of the structure so that parallel computation of nullspace basis matrix is easy. The motivation leads to the definition for a proper partition.

DEFINITION 2. Let $\mathcal{S} = (\mathcal{N}, \mathcal{E})$ be a structure and consider the collection of pairs $\{(\mathcal{N}_k, \mathcal{E}_k) : \mathcal{N}_k \subseteq \mathcal{N}, \mathcal{E}_k \subseteq \mathcal{E}, 1 \leq k \leq K+1\}$, then the collection is called a *partition* of $\mathcal{S}$ if

(i) $\mathcal{N} = \cup_{k=1}^{K+1} \mathcal{N}_k$ is a disjoint union,

(ii) $\mathcal{E} = \cup_{k=1}^{K+1} \mathcal{E}_k$, and the first K sets $\mathcal{E}_k$ are disjoint, and

(iii) $(\mathcal{N}_k, \mathcal{E}_k)$ are substructures for $1 \leq k \leq K$.

DEFINITION 3. Let $\{\mathcal{S}_k = (\mathcal{N}_k, \mathcal{E}_k) | k = 1, \cdots, K+1\}$ be a partition of $\mathcal{S}$=$(\mathcal{N}, \mathcal{E})$. A partition is called *proper* if

(i) $\mathcal{N}_{K+1}$ is empty,

(ii) $\mathcal{N}_k$ and $\mathcal{E}_k$ have the same cardinalities for $1 \leq k \leq K$,

(iii) $\mathcal{S}_k$ are stable for $k = 1, \cdots, K$; that is, each block E_k of E has an inverse.

We remark that the equilibrium matrix E for Figure 1. with a proper partition has the following form.

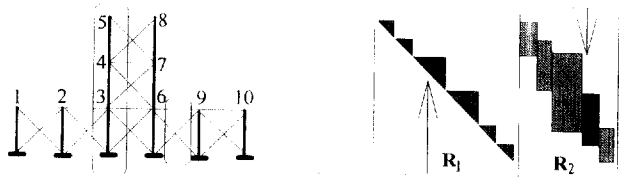


FIGURE 2: 6 Disjoint Stable Substructures and its Equilibrium Matrix

Each upper triangular diagonal block has an inverse, and corresponds to stable substructures given by $\mathcal{S}_1 = (\{1\}, \{e_1\}), \cdots, \mathcal{S}_3 = (\{3,4,5\}, \{e_3, e_4, e_5\}), \cdots, \mathcal{S}_6 = (\{10\}, \{e_{10}\})$. The remaining elements, $e_{11}, \cdots, e_{31}$, connect these stable substructures. Note that the diagonal structure of R_2 which is a result of ordering the connecting elements from the left to the right. Because of this structure of R_2, we can also do a lot of work in parallel computation of $R_1^{-1}R_2$.

We present an example used to test the effectiveness of substructure scheme with proper partitions in parallel computations. The following calculations for each example were done on the Alliant FX/8 at Argonne National Laboratory. The Alliant FX/8 has 8 processor nodes(called CEs or computational elements) with vector instruction. Parallelism may be achieved by using compiler directives. The parallelism is loop based with the inner loops dedicated to the vector instructions and the outer loops dedicated to CEs. Various compiler directives can be used to control the amount of parallelism.

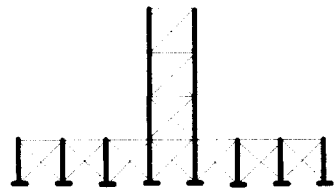
$-Og$	Optimized Serial
$-Ogv$	Optimized Vector
$-Ogc-c\#$	Optimized Concurrent with # of processors
$-O$	Optimized Concurrent with Vector

We suppressed vectorization because it couldn't give a decrease in time due to data dependency in back substitution. Following two ex-

amples indicate very good effeciencies of using substructure with proper partition on parallel computation. Here speedup is defined as follows

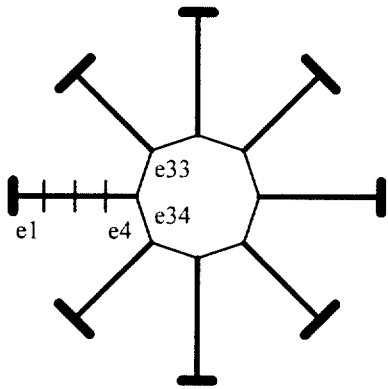
$$\text{Speedup} = \frac{\text{time for } -Ogc - c\# \text{ calculations}}{\text{time for } -Og \text{ calculations}}.$$

EXAMPLE 2. This example of a pin-jointed-structure with 14 nodes and 44 elements, and the matrix E is 28×88.



Directive	Time	Speedup
$-Og$	$6.81E$-02	1.00
$-Og_c$ $-c_2$	$1.61E$-02	1.95
$-Og_c$ $-c_4$	$8.59E$-03	3.66
$-Og_c$ $-c_8$	$5.08E$-03	6.20

EXAMPLE 3. Consider a rigid frame which models a wheel with 8 spokes. Each spoke is a stable substructure and together they form a proper partition. The connecting elements are indicated by the light lines $e_{33}, \cdots, e_{40}$. The matrix E is 96×120.



Directive	Time	Speedup
$-Og$	$6.87E$-02	1.00
$-Og_c$ $-c_2$	$3.57E$-02	1.92
$-Og_c$ $-c_4$	$1.78E$-02	3.86
$-Og_c$ $-c_8$	$9.68E$-03	7.10

3. Application to Incompressible Fluid Flow

In this section we consider an application of the substructuring method with proper partition 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 F will change a little from one time step to next in fluid case. As E reflects the conservation of mass equation, E 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.

EXAMPLE 4. (Driven Cavity)

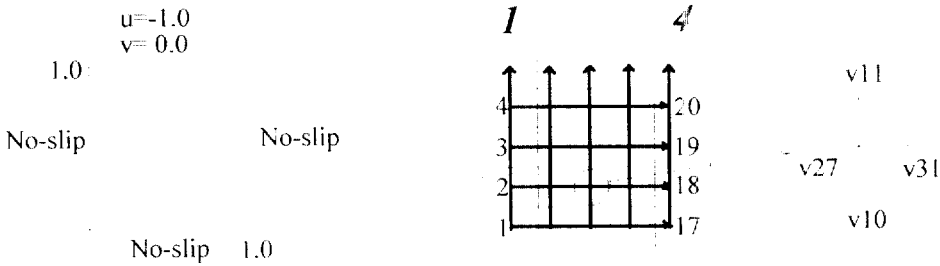


FIGURE 3:
Driven Cavity and its Finite Difference Grid with Substructure

A finite difference grid with 20 cells has 36 unknown velocity components is illustrated in Figure 3. 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 [hall]. Consider the proper partition of a finite difference grid as in Figure 3.

Each substructure is stable, and then the associated equilibrium matrix E has the following form:

$$\left[\begin{array}{ccccc|cccccc} f & & & & & i & & & & & \\ & f & & & & -i & i & & & & \\ & & f & & & & -i & i & & & \\ & & & f & & & & -i & i & & \\ & & & & f & & & & -i & i & \\ & & & & & & & & & -i & \end{array}\right],$$

where $f = \begin{bmatrix} 1 & & & \\ -1 & 1 & & \\ & -1 & 1 & \\ & & -1 & 1 \end{bmatrix}$, $i = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{bmatrix}$

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

$$\frac{v_{31} - v_{27}}{h} + \frac{v_{11} - v_{10}}{h} = 0,$$

where $h = \Delta x = \Delta y$.

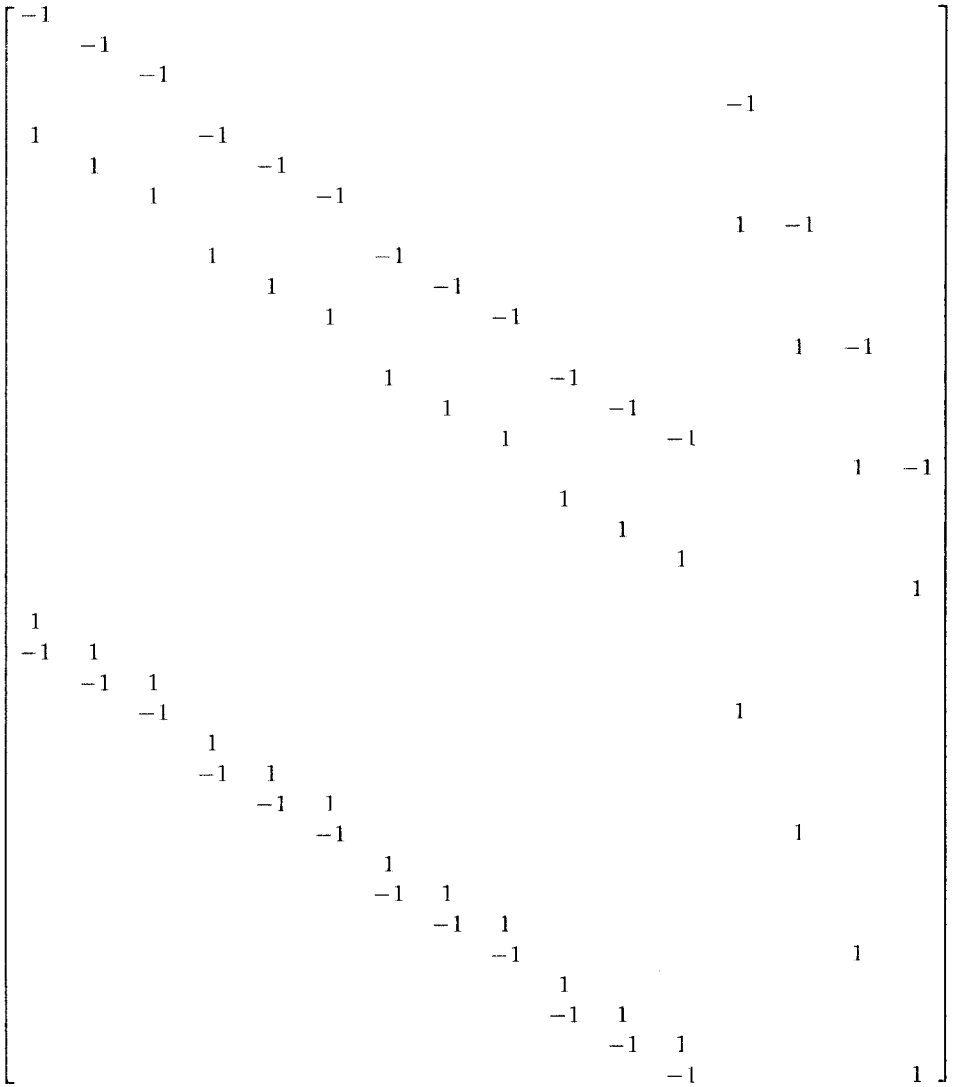
The resulting nullspace basis matrix N has the form:

$$N = \begin{bmatrix} f^{-1} & & & & \\ -f^{-1} & f^{-1} & & & \\ & -f^{-1} & f^{-1} & & \\ & & -f^{-1} & f^{-1} & \\ & & & -f^{-1} & \\ & & -I & & \end{bmatrix}, \quad \text{where } f^{-1} = \begin{bmatrix} 1 & & & \\ 1 & 1 & & \\ 1 & 1 & 1 & \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

The matrix N also can be expressed as product of N' and F, where

$$N'F = \begin{bmatrix} i & & & & \\ -i & i & & & \\ & -i & i & & \\ & & -i & i & \\ & & & -i & \\ -f & & & & \\ & -f & & & \\ & & -f & & \\ & & & -f & \end{bmatrix} \begin{bmatrix} f^{-1} & & & \\ & f^{-1} & & \\ & & f^{-1} & \\ & & & f^{-1} \end{bmatrix}.$$

It is interesting to compare this nullspace basis with the basis, $\overline{N}$, obtained in Hall [8] by using graph theoretic ideas. The nullspace basis in Hall [8], $\overline{N}$, has the following form:



By interchanging columns 4, 8 and 12 with 13, 14 and 15, respectively, result in a transformation of N' is exactly same as $-\overline{N}$. $\overline{N}$ is more sparse, but $\overline{N}$ may not be constructed by utilizing the properties of a proper partition. We can extend all of the discussion we made for the 2-dimension driven cavity problem to the 3-dimension case.

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