A Split Operator Method for Transient Problems

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ABSTRACT

Numerous techniques have been developed for improving the computational efficiency of transient analysis: mesh partitioning [1-4], subcycling procedures [5-7] and operator splitting methods [8-9]. In mesh partitioning methods, the model is divided into subdomains which are integrated by different time integrators, typically implicit and explicit. Any stiff portions of the model are integrated by the implicit operator so that the size of the time step can be increased. In subcycling procedures, the stiff portions are integrated by smaller time steps, yielding similar benefits.

However, in models for which the governing partial differential equations are basically of a parabolic character, explicit methods can become quite expensive for refined models because the size of the stable time step decreases with the square of the minimum element dimension. Thus explicit methods, whether employed alone or with partitioning or subcycling, have inherent limitations in these problems.

A new procedure is here described for the element-by-element semi-implicit method of Hughes and coworkers which requires the solution of only small systems of equations. This procedure is described for a family of uniform gradient or strain elements which are widely used in nonlinear transient analysis. The diffusion equation and the equations of motion for both shells and continua have been treated, but only the former is considered herein. Results are presented for several examples which show the potential of this method for improving the efficiency of a large-scale linear and nonlinear computations.

INTRODUCTION

Hughes and coworkers [10, 11] have recently presented a novel splitting scheme ideally suited for finite elements which involves only the inversion of the individual element matrices. The scheme is easily applied to arbitrary combinations of elements and node numbers. However, although the requirement of only element inversion seems benign at first, it poses a substantial drawback. Consider that the simplest quadrilateral shell element has 24 degrees of freedom, and that 8 to 20 inversions of each element must be made in each time step; the number of computations for a large mesh is then quite large. Although the element inverses are sometimes stored, this is impractical in nonlinear problems, where the inverse changes with the evolution of the problem and furthermore requires considerable storage.

In this paper, a method is developed for inverting the element equations by solving a much smaller system of equations. The method is based on certain orthogonality conditions developed in [12]. The method has been applied to the following elements: i) 3 node triangle in two dimensions; ii) 4 node quadrilateral in two dimensions; iii) 4 node tetrahedron in three dimensions; iv) 8 node hexahedron in three dimensions; v) 4 node shell element in three dimensions. These elements are shown in Fig. 1. All of these elements are examples of the "uniform" strain elements developed in [12], and are the elements which are most widely used in nonlinear, transient analysis. In three dimensions the reduction in computations is quite significant. For example, for the 8 node hexahedron, this method requires the solution of a 9 x 9 system instead of a 24 x 24 system. Since the cost of solving a full system such as this varies with N^3, its cost is 5% of that of the original method. In the next section, the method is illustrated for the diffusion equation in two and three dimensions. Some examples of solutions by this method are given in Section 3.

I. APPLICATION TO DIFFUSION EQUATION

The spatially discretized form of the diffusion equation is

$$\underset{\sim}{M}\,\dot{\underset{\sim}{u}} + \underset{\sim}{K}\,\underset{\sim}{u} = \underset{\sim}{s} \tag{1}$$

where $\underset{\sim}{M}$ is the capacitance matrix, which is assumed to be diagonal, $\underset{\sim}{u}$ the matrix of nodal temperatures and $\underset{\sim}{s}$ the matrix of nodal sources; a superposed dot designates a time derivative. An implicit integrator which is unconditionally stable for first-order ODE's is the trapezoidal rule (Crank-Nicolson)

$$\underset{\sim}{u}^{n+1} = \underset{\sim}{u}^{n} + \frac{1}{2}\Delta t\,(\dot{\underset{\sim}{u}}^{n} + \dot{\underset{\sim}{u}}^{n+1}) \tag{2}$$

where superscripts designate the step number and Δt the time step.

When Eq. (2) is combined with Eq. (1), the following equation is obtained for $\underset{\sim}{u}^{n+1}$ in terms of the historical values of the variable

$$(\underset{\sim}{M} + \frac{1}{2}\Delta t\,\underset{\sim}{K})\,\underset{\sim}{u}^{n+1} = (\underset{\sim}{M} - \frac{1}{2}\Delta t\,\underset{\sim}{K})\,\underset{\sim}{u}^{n} + \frac{1}{2}\Delta t(\underset{\sim}{s}^{n} + \underset{\sim}{s}^{n+1}) = \underset{\sim}{M}\,\underset{\sim}{f} \tag{3}$$

Premultiplying the above by $\underset{\sim}{M}^{-1}$ yields

$$(\underset{\sim}{I} + \frac{1}{2}\Delta t\ \underset{\sim}{M}^{-1}\ \underset{\sim}{K})\ \underset{\sim}{u}^{n+1} = \underset{\sim}{f} \tag{4}$$

where $\underset{\sim}{I}$ is the unit matrix.

The essential idea of the Hughes' method is that the summation of the element stiffnesses implicit within the assembly $\underset{\sim}{K}$ from the n_e element stiffnesses $\underset{\sim}{K}^{(e)}$ is approximated by a product, so that

$$\underset{\sim}{I} + \frac{1}{2}\Delta t\ \underset{\sim}{M}^{-1}\ \underset{\sim}{K} = \underset{\sim}{I} + \frac{1}{2}\Delta t\ \underset{\sim}{M}^{-1}\ \sum_{e}^{n_e} \underset{\sim}{K}^{(e)} \tag{5}$$

is approximated by

$$\underset{\sim}{I} + \frac{1}{2}\Delta t\ \underset{\sim}{M}^{-1}\ \sum_{e}^{n_e} \underset{\sim}{K}^{(e)} = \prod_{e}^{n_e} (\underset{\sim}{I} + \frac{1}{2}\Delta t\ \underset{\sim}{M}^{-1}\ \underset{\sim}{K}^{(e)}) \tag{6}$$

where $\prod$ is the product operator. If $\underset{\sim}{G}^{(e)}$ is defined by

$$\underset{\sim}{G}^{(e)} = \underset{\sim}{I} + \frac{1}{2}\Delta t\ \underset{\sim}{M}^{-1}\ \underset{\sim}{K}^{(e)} \tag{7}$$

then Eqs. (4) become

$$(\prod_{e}^{n_e}\ \underset{\sim}{G}^{(e)})\ \underset{\sim}{u}^{n+1} = \underset{\sim}{f} \tag{8}$$

Since $\underset{\sim}{K}^{(e)}$ is nonzero only over the nodes of the element, Eq. (8) can be replaced by a sequence of equations

$$\underset{\sim}{G}^{(e)}\ \underset{\sim}{u}^{(e)} = \underset{\sim}{f}^{(e)} \qquad e = 1 \text{ to } n_e \tag{9}$$

where the time-step superscripts are dropped for convenience. Each equation is a linear algebraic system of n_N equations in n_N unknowns, where n_N is the number of nodes per element. Thus the method is independent of bandwidth.

Remark 1. The relevant part of $\underset{\sim}{M}$ can usually be approximated by a scalar multiple of the unit matrix, $\rho\ \underset{\sim}{I}$, so that $\underset{\sim}{G}^{(e)}$ can be approximated by

$$\underset{\sim}{G}^{(e)} = \underset{\sim}{I} + \overline{\gamma}\ \underset{\sim}{K}^{(e)} \qquad \overline{\gamma} = \frac{\Delta t}{2\rho} \tag{10}$$

Remark 2. Rather than sweeping simply from 1 to n_e, it is useful to sweep over the operator $\underset{\sim}{G}^{(e)}$ several times, alternately reversing the sweep, so that the sweeps are 1 to n_e, n_e to 1, etc.

Remark 3. The results of these sweeps may be considered an estimate to $\underset{\sim}{u}$ as in a split operator method, so that (9) can be combined with iterative acceleration methods.

The element conductance matrix for anisotropic diffusion is given by

$$K_{IJ}^{(e)} = \int_{\Omega_{(e)}} N_{I,i}\ k_{ij}\ N_{J,j}\ d\Omega \tag{11}$$

where N_I are the shape functions, $\Omega_{(e)}$ is the domain of the element (the area A or the volume V in two and three dimensions, respectively) and k_{ij} the conductivity matrix. Standard indicial notation is used. If one point quadrature is used to evaluate $\underset{\sim}{K}^{(e)}$, we obtain

$$\underset{\sim}{K}^{(e)} = \Omega^{-1} k_{ij} \underset{\sim}{b}_i \underset{\sim}{b}_j^T \tag{12a}$$

where the vectors $\underset{\sim}{b}_i$ are rows of a $\underset{\sim}{B}$ matrix defined as follows

$$B_{iI} = N_{I,i} (\underset{\sim}{x}_Q) \tag{12b}$$

where $\underset{\sim}{x}_Q$ is the quadrature point. The matrix $\underset{\sim}{G}^{(e)}$ as given by Eq. (10) becomes

$$\underset{\sim}{G}^{(e)} = \underset{\sim}{I} + \gamma k_{ij} \underset{\sim}{b}_i \underset{\sim}{b}_j^T \qquad \gamma = \overline{\gamma}/\Omega \tag{13}$$

For purposes of clarity, the method will first be presented for the two dimensional quadrilateral element. The vectors $\underset{\sim}{b}_i$ are then given by

$$\underset{\sim}{b}_1^T = \frac{1}{2} [y_{24}, y_{31}, y_{42}, y_{13}] \qquad \underset{\sim}{b}_2^T = \frac{1}{2} [x_{42}, x_{13}, x_{24}, x_{31}] \tag{14a}$$

$$x_{IJ} = x_I - x_J \qquad y_{IJ} = y_I - y_J \tag{14b}$$

where x_I and y_I are the coordinates of the nodes. Two additional vectors are defined

$$\underset{\sim}{s}_1^T = [1, 1, 1, 1] \qquad \underset{\sim}{s}_2^T = [1, -1, 1, -1] \tag{15}$$

The following results first given in [12] are needed for this development:

(i) the vectors $\underset{\sim}{b}_i$ are orthogonal to $\underset{\sim}{s}_i$, and $\underset{\sim}{s}_i$ are orthogonal to each other so that $\underset{\sim}{b}_i$ and $\underset{\sim}{s}_i$ span the space R^4 and

$$\underset{\sim}{b}_i^T \underset{\sim}{s}_j = 0 \qquad \underset{\sim}{s}_i^T \underset{\sim}{s}_j = \eta_N \delta_{ij} \tag{16}$$

(ii) the vectors of nodal coordinates $\underset{\sim}{x}_1^T \equiv \underset{\sim}{x} = [x_1, x_2, x_3, x_4]$, $\underset{\sim}{x}_2^T \equiv \underset{\sim}{y} = [y_1, y_2, y_3, y_4]$ are dual to $\underset{\sim}{b}_i$, so that

$$\underset{\sim}{x}_i^T \underset{\sim}{b}_j = \underset{\sim}{b}_j^T \underset{\sim}{x}_i = A \delta_{ij} \tag{17}$$

where δ_{ij} is the Kronecker delta; because of this duality $\underset{\sim}{x}_i$ and $\underset{\sim}{s}_i$ also span the space R^4.

The solution of Eqs. (9) is performed as follows. Since $\underset{\sim}{x}_i$ and $\underset{\sim}{s}_i$ span R^4, it follows that any solution for the element nodal variables can be written in the form

$$\underset{\sim}{u}^{(e)} = \alpha_k \underset{\sim}{x}_k + \beta_\kappa \underset{\sim}{s}_\kappa \tag{18}$$

Substituting Eqs. (13) and (18) into (9) and premultiplying by $\underset{\sim}{b}_j^T$, it follows from the orthogonality properties that

$$\alpha_k \left(\delta_{jk} + \gamma\, k_{ik}\, \underset{\sim}{b}_j^T\, \underset{\sim}{b}_i\right) = \frac{1}{A}\, \underset{\sim}{b}_j^T\, \underset{\sim}{f}^{(e)} \tag{19}$$

If Eq. (9) is now premultiplied by $\underset{\sim}{s}_j^T$, the orthogonality properties yield

$$\beta_\kappa = \frac{1}{n_N} \left(\underset{\sim}{s}_\kappa^T\, \underset{\sim}{f}^{(e)} - \alpha_i\, \underset{\sim}{s}_\kappa^T\, \underset{\sim}{x}_i\right) \tag{20}$$

where n_N is the number of nodes per element, which is 4 for the quadrilateral.

Equation (19) is a system of 2 equations in 2 unknowns, and once $\underset{\sim}{\alpha}$ is known, $\underset{\sim}{\beta}$ can be evaluated directly without the solution of any equations. The solution is then obtained by simply substituting into Eq. (18). Thus this procedure replaces the solution of 4 equations in 4 unknowns by a system of 2 equations. In addition, it is worth noting that: 1) the stiffness matrix $\underset{\sim}{K}^{(e)}$ need never be computed; 2) many of the operations indicated in Eq. (20) as matrix multiplications are simply vectors sums since the terms of $\underset{\sim}{s}_i$ are always ± 1.

For three dimensional problems, the conductance matrix is also given by Eq. (12a). The $\underset{\sim}{b}_i$ and $\underset{\sim}{s}_i$ matrices are taken from [12]. The solution for any element is again approximated by Eq. (18) with a range of 4 on the Greek subscripts. Equations (19) and (20) follow as before. The solution process now involves a 3 x 3 system rather than an 8 x 8 system.

III. EXAMPLES

Thermal problems, which are isotropic and linear, were solved. All parameters are expressed in dimensionless form; the thermal diffusivity is given by

$$a = \frac{k}{\rho c} \qquad \bar{t} = t/T \qquad \bar{\ell} = \ell/L \qquad \bar{a} = a\, T/L^2 \tag{21}$$

where the above are dimensionless time, length, and diffusivity, ρ and c are the density and thermal capacitance; T and L are the units of time and distance, respectively. Where a critical time step is cited, it refers to the maximum stable time step for an Euler explicit integrator. The circular domain with an insulated boundary (the normal derivative of u vanishes along the boundary) shown in Fig. 2 was used. The initial conditions are $u(\underset{\sim}{x},0) = 0$. A heat source with the time history shown in Fig. 2 was applied at the center, node 1.

The problem was first solved with uniform properties $\bar{a} = 0.04$. Table 1 shows the average number of sweeps required for solving the problem.

The following observations can be made from Table 1: 1) the number of iterations seems to grow slowly with increasing time step and sometimes even decrease; 2) the number of iterations is quite sensitive to the tolerance; 3) the number of iterations is substantially below the number of time steps which would be required in an explicit method.

The study was repeated using the same time steps with the dimensionless thermal diffusivities in zones 1 to 4 given by 50, 4, 0.04 and 0.8, respectively; the zones are indicated in Fig. 2. In this case, the stable explicit time step is 0.02 that for the previous case because of the large increase in the thermal diffusivity of zone 1. The number of iterations required increased only by 50% when the same time steps were used.

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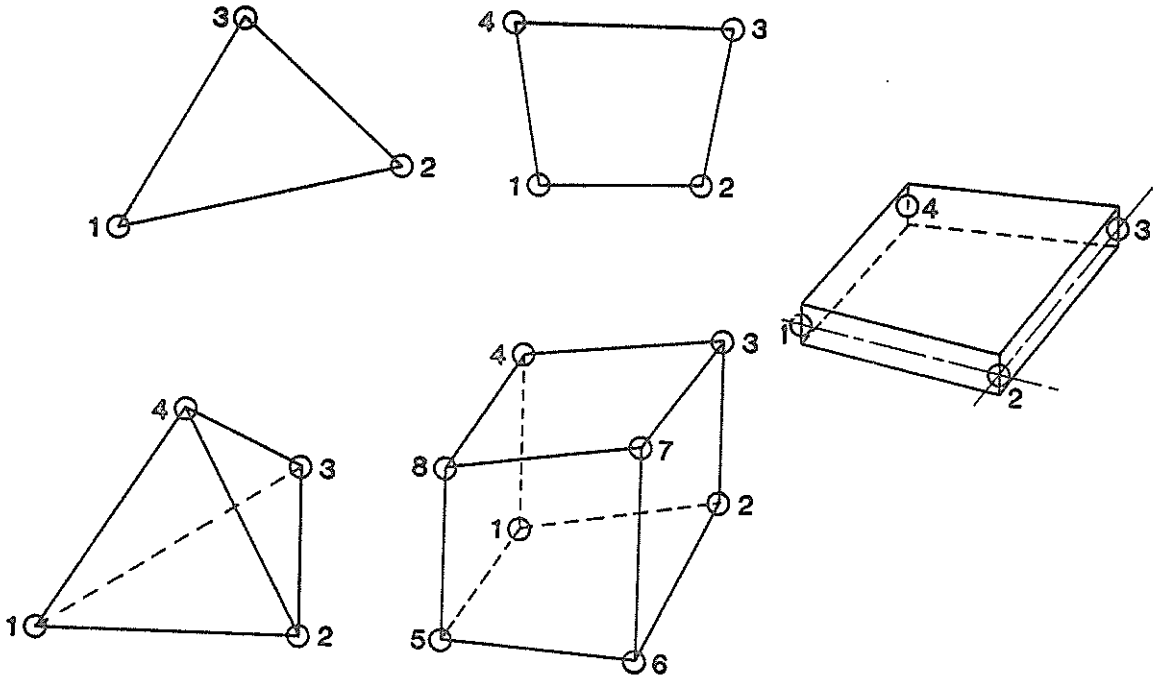

Figure 1. Family of uniform gradient and uniform strain elements: (1) triangle; (2) tetrahedron; (3) 4 node quadrilateral; (4) 8 node hexahedron; (5) 4 node plate/shell element.

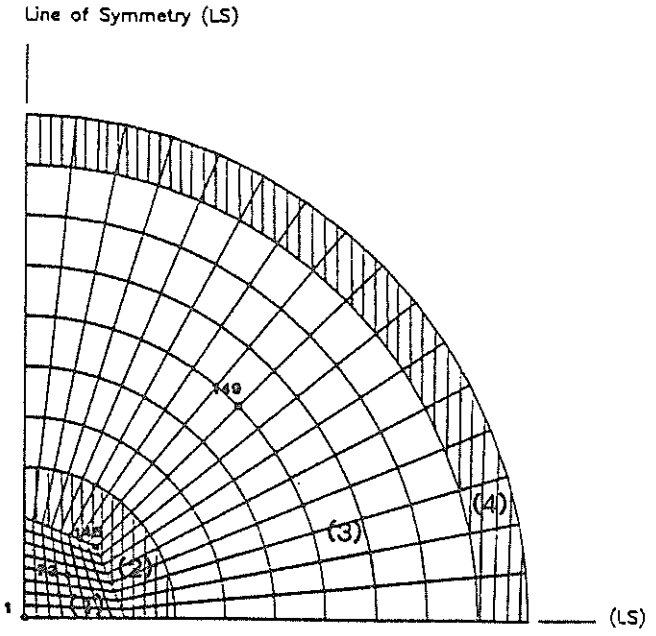

Figure 2. Mesh for example.

Table 1. Number of iterations (sweeps) required per time step in example 1

$\Delta t/\Delta t_{crit}$	20		30		100	
ε^*	10^{-3}	10^{-2}	10^{-3}	10^{-2}	10^{-3}	10^{-2}
Number of iterations						
Maximum	7	6	7	5	13	15
Minimum	5	4	4	3	8	6
Average	6.1	4.6	5.3	3.8	6.4	5.1

*ε is the energy tolerance defined in Ref. [13]