A Consistent Linearization Method for Finite Element Analysis of Viscoelastic Materials

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SUMMARY

A method of formulating material models for viscoelastic analysis using the finite element method is presented. The method, named consistent linearization, includes the influence of creep in the material stiffness in a theoretically ideal manner.

A common approach for solving creep problems is the initial strain method, in which the stiffness matrix is elastic and the effect of creep is included only in the unknown force term. More rapid convergence can be achieved and longer time steps can be employed by including the effect of creep in the stiffness matrix. In some previous works creep has been considered approximately. Errors in the approximation have been corrected by equilibrium iteration, using stresses compnted with a more accnrate integration. In this paper, additional improvement is achieved by formulating the stiffness and the stress consistently. This not only ensures an optimum convergence rate, but it avoids the cost of unnecessarily accurate stress computations in cases for which the solntion error is dominated by the global time discretization.

In the consistent linearization method the tangent material stiffness is defined as the partial derivative (or Jacobian matrix) of the end-of-step stress with respect to the strain increment applied over a constant time interval. The material stiffness is calculated using a numerical integration scheme which is identical to that used for calculating the end-of-step stress. When the stress and the stiffness are consistent, the equilibrium iteration becomes a pure Newton's method. A linear viscoelastic material is treated as truly linear, and in this case the time integration can be performed withont equilibrium iteration. The same approach can be used to linearize a nonlinear material.

This method has been applied to the linear viscoelastic analysis of graphite snbject to irradiation. Previously, using the initial strain method, short time steps had been required to avoid a numerical instability associated with the rapid transient creep. Using the consistent linearization method a factor of 15 reduction in computer time was achieved for the same accuracy.

1. Introduction

This work was motivated by the need to calculate stresses in the graphite fuel element (Fig. 1) of a High Temperature Gas Cooled Reactor. Graphite under irradiation may be treated as a linear viscoelastic material and idealized with the Maxwell-Kelvin model [1] shown in Fig. 2. Owing to the geometrical complexity and time dependence of the problem, computational efficiency has been a matter of great interest [2].

Most well-known finite element codes have evolved to use the same basic computational algorithm, known as the tangent stiffness method with equilibrium iteration [3, 4, 5]. Within this framework, numerous algorithms have been developed for defining the nodal point stiffness and calculating the element stress, from which the equilibrium error vector is determined. The approach taken here is to define the stiffness and the stress consistently. This, we believe, leads to an optimum rate of convergence of the equilibrium iteration.

To solve large problems efficiently, GA Technologies recently developed a finite element program named TWOD. TWOD employs higher order isoparametric elements, efficient data processing, and a general purpose material model interface [6]. The solution driver assumes a piecewise linear strain path, and it employs flexible procedures for matrix updates and equilibrium iteration. The material interface permits the constitutive law to be linearized arbitrarily by the user and the stress to be computed by a user-defined integration procedure.

In the first attempt to use TWOD for a graphite analysis, the initial strain method was employed. The stiffness matrix was elastic, and the creep strains were considered as contributions to force (for prediction) or the stress for equilibrium iteration. The stresses were calculated from the total strain increments using a one-step, explicit, fourth order Runge Kutta method. This attempt failed when it has observed that the explicit integration introduced a numerical instability. The critical time step was severely restrictive, increasing the number of time steps required from around 36 (needed for accuracy) to around 800 (needed for stability). Similar results have been observed and diagnosed by Cormeau [7].

A number of improved solution algorithms for nonlinear materials have been desribed in the literature. In [8] and [9] the influence of nonlinearity is included in the stiffness matrix through a technique based on a forward difference, first order Taylor series. In [10] and [11] implicit stiffness matrices are derived by introducing scalar integration parameters, similar in concept to the Wilson θ or Crank-Nicholson methods. None of these approaches considers in detail the intimate relationship that exists between the stiffness and the stress.

To obtain more insight into the numerical instability, a one-dimensional version of the equilibrium iteration algorithm was studied. This study, summarized below, demonstrated that there is a preferred definition of the material stiffness based on the true Jacobian matrix of the end-of-step equilibrium equations. It also disclosed that a rapid rate of convergence is achieved when the stiffness matrix and the stress are calculated using exactly the same integration procedure.

This method, termed consistent linearization, is illustrated herein for a linear viscoelastic model of graphite. With this method, a linear viscoelastic material is treated as truly linear, i.e., equilibrium iteration is unnecessary. Nonlinear materials can be linearized similarly, using equilibrium iteration to correct for nonlinearity.

2. One-Dimensional Study

The finite element stiffness method is essentially a procedure for mapping between a local constitutive law, considered at the element integration point level, and the global stiffness equations, which combine the local influences. Each step of the equilibrium iteration consists of an alternation between local and global calculations. If one were to study this process in detail, the algebra would be complicated by the mapping relationships. This is avoided here by considering a one-dimensional problem consisting of a bar with unit area and unit length. For this case the local and global quantities are scalars and are identical.

Assume that the externally applied stress is given as a function of time, $\sigma_e(t)$. The object is to calculate the internal stress, $\sigma(t)$, and strain, $\varepsilon(t)$. The equilibrium equation for the finite element problem is given by the well-known relationship [5],

$$\int_V [B]^T \{\sigma(t)\}\, dV - \{F(t)\}] = \{0\} \quad , \tag{1}$$

which reduces in this example to the trivial equation,

$$\sigma(t) - \sigma_e(t) = 0. \tag{2}$$

One may ignore the fact that $\sigma(t)$ is known through Eq. (2) and proceed to compute $\sigma(t)$ using the equilibrium iteration method.

At the start of each time interval the stress and strain are known. It is assumed that the unknown strain increment, $\Delta\varepsilon$, is applied linearly over the time interval Δt. The end of step stress, σ, is obtained by integrating the constitutive law, giving

$$\sigma = h(\Delta\varepsilon, \Delta t) \quad . \tag{3}$$

In view of Eq. (3), the equilibrium condition at the end of the step may be written as

$$f(\Delta t) = \sigma(\Delta\varepsilon) - \sigma_e = 0. \tag{4}$$

Here f is the unbalanced force (stress) caused by a failure to satisfy equilibrium.

The unknown strain increment, $\Delta\varepsilon$, is calculated by applying Newton's method to find the root of the function f. The algorithm is begun by making a first guess for the strain increment, either as zero or by extrapolation from previous strain rates. Then, for a typical iteration i, the next guess for the strain increment is given by

$$\Delta\varepsilon_{i+1} = \Delta\varepsilon_i + \delta\varepsilon_i \quad , \tag{5}$$

where

$$\delta\varepsilon_i = \frac{-f(\Delta\varepsilon_i)}{\dfrac{\partial f(\Delta\varepsilon_i)}{\partial\Delta\varepsilon}} \tag{6}$$

Observe that

$$\frac{\partial f}{\partial\Delta\sigma} = \frac{\partial\sigma}{\partial\Delta\varepsilon} = D, \tag{7}$$

where

$$D \equiv \left.\frac{\partial h(\Delta\varepsilon,\Delta t)}{\partial \Delta\varepsilon}\right|_{\substack{\Delta\varepsilon = \Delta\varepsilon_i \\ \Delta t = \text{given}}} \quad . \tag{8}$$

For a viscoelastic material, D is the creep stiffness, representing the perturbation of the end-of-step stress that is incurred through a perturbation of the incremental strain.

Now consider that the stress used to determine the unbalanced force f may be computed approximately as $\sigma^*(\Delta\varepsilon_i)$ by numerical integration of the constitutive law. Also, consider that the material stiffness D may be approximated as $\tilde{D}$ say, using values from a previous time step or perhaps even the elastic stiffness.

With these approximations, Eqs. (4), (6), and (7) may be combined to give

$$\delta\varepsilon_i = \frac{1}{\tilde{D}} \left(\sigma_e - \sigma^*(\Delta\sigma)\right)_i \quad . \tag{9}$$

To evaluate the convergence characteristics of this iteration, two successive iterates are examined. From (5) and (9) one obtains

$$\frac{\delta\varepsilon_{i+1}}{\delta\varepsilon_i} = 1 - \frac{1}{\tilde{D}} \left(\frac{\sigma^*(\Delta\varepsilon_i + \delta\varepsilon_i) - \sigma^*(\Delta\varepsilon_i)}{\delta\varepsilon_i} \right) \quad . \tag{10}$$

From the definition of a derivative, it follows that if $\delta\varepsilon_i$ is small compared with $\Delta\varepsilon_i$,

$$\frac{\delta\varepsilon_{i+1}}{\delta\varepsilon_i} \approx 1 - \frac{D^*}{\tilde{D}} \quad , \tag{11}$$

where

$$D^* \equiv \left.\frac{\partial \sigma^*(\Delta\varepsilon)}{\partial \Delta\varepsilon}\right|_{\substack{\Delta\varepsilon = \Delta\varepsilon_i \\ \Delta t = \text{given}}} \quad . \tag{12}$$

D^* is the Jacobian of the incremental, numerically integrated constitutive law. According to Eq. (11) the convergence rate is a maximum when

$$\tilde{D} = D^* \quad . \tag{13}$$

This is the crux of the consistent linearization method.

Although consistent linearization ensures rapid convergence of the equilibrium iteration, it does not guarantee accuracy or stability of the forward marching process. This is governed by characteristics of the time integration itself. The benefit of using the consistent linearization method is that unnecessary iterations to compensate for inconsistencies in the material stiffness are eliminated, so the efficiency of the solution is governed solely by the choice of the integration algorithm and the length of the time step.

3. Calculation of the Material Stiffness

A straightforward way to calculate the material stiffness D^* is to integrate along a trial strain path and to perturb the strain path one component at a time, re-integrating to determine the stress perturbation. Each perturbation gives a column of the Jacobian matrix, i.e.,

$$D^*_{ij} \equiv \frac{\partial \sigma^*_i}{\partial \varepsilon_j} \sim \frac{\sigma^*_i (\varepsilon + \delta\varepsilon_j) - \sigma^*_i (\varepsilon)}{\delta\varepsilon_j} \quad . \tag{14}$$

For nonlinear materials this method has one shortcoming in that the size of the perturbation required to obtain both numerical significance and accuracy is unknown.

A better procedure in some cases is to perturb the constitutive law algebraically. The result is a linearized system of equations having a constant Jacobian such that the size of the perturbation is irrelevant. For a linear viscoelastic material, these two approaches are essentially the same.

4. Implementation for a Linear Viscoelastic Material

In the following, the consistent linearization method is implemented for the Maxwell-Kelvin model shown in Fig. 2. All lower case letters are vectors, with stress σ and strain ε having length 6. Upper case letters are matrices, e.g., 6 x 6.

The equations for the four strain components of the model are:

Elastic $$\varepsilon^E = (E^E)^{-1} \sigma, \tag{15}$$

Steady Creep $$\dot{\varepsilon}^S = M^S \sigma, \tag{16}$$

Transient Creep $$\dot{\varepsilon}^T = M^T (\sigma - E^T \varepsilon^T), \tag{17}$$

Thermal/Irradiation $$\varepsilon^\theta = \varepsilon^\theta(t) \qquad \text{(given)}, \tag{18}$$

where the dot ($\cdot$) means differentation with respect to fast neutron fluence. Eqs. (15) (18) are coupled by

$$\varepsilon = \varepsilon^E + \varepsilon^S + \varepsilon^T + \varepsilon^\theta \quad . \tag{19}$$

With a suitable combination of the above, one obtains a system of 12 first order, ordinary differential equations,

$$\{\dot{x}\} = - [A] \{x\} + \{b\} \quad , \tag{20}$$

where

$$\{x\} \equiv \begin{Bmatrix} \varepsilon^E \\ \varepsilon^T \end{Bmatrix} \quad , \quad \{b\} = \begin{Bmatrix} \dot{\varepsilon} - \dot{\varepsilon}^\theta \\ 0 \end{Bmatrix}$$

and

$$[A] = \begin{bmatrix} (M^S + M^T)E^E & - M^T E^T \\ - M^T E^E & M^T E^T \end{bmatrix} \tag{21}$$

To integrate the system, Eq. (20), a variant of the Crank-Nicholson implicit method is used. This scheme was chosen because the critical time step was too restrictive with an explicit method. Therefore, either an explicit integration with many substeps or an implicit integration would have been required to handle long time steps. Both were tried and, as will be shown below, the implicit method was more efficient.

The integration algorithm is described by

$$\Delta x = [(1 - \theta)(-A_1 x_1 + b_1) + \theta(-A_2 x_2 + b_2)] \Delta t, \tag{22}$$

where the subscripts 1 and 2 refer to the start and end of the step. Given that $b_1 = b_2 =$ constant and $x_2 = x_1 + \Delta x$, Eq. (22) can be written as

$$[I + \theta \Delta t A_2] \Delta x = \{-[(1 - \theta)A_1 + \theta A_2] x_1 + b\} \Delta t \quad . \tag{23}$$

To reduce the number of material property calculations, Eq. (23) is simplified by evaluating the matrix A only at time $t_1 + \theta \Delta t$. Call this matrix A_θ. Then (23) reduces to

$$[I + \theta \Delta t A_\theta] \Delta x = (-A_\theta x_1 + b) \Delta t \quad . \tag{24}$$

After its assembly, the matrix $[I + \theta \Delta t A_\theta]$ is factored using the Cholesky method, and the matrix factors are stored for future operations.

To find the stresses at the end of the step, the system (24) is solved for Δx, and the stresses are calculated by

$$\sigma_2 = \sigma_1 + E^E \Delta \varepsilon^E \quad . \tag{25}$$

The material stiffness is calculated by a perturbation of Eq. (24). Since A_θ and x_1 are constant but Δx and b may vary, the perturbed system is

$$[I + \theta \Delta t A_\theta] \delta \Delta x = \delta b \Delta t \quad . \tag{26}$$

If Eq. (26) is solved six times (j = 1 to 6), perturbing one strain component each time, such that

$$(\delta b_j)_i = \frac{\delta_{ij} \text{ (Kroneker delta)}}{\Delta t} \quad , \tag{27}$$

the resulting stress increment,

$$\delta \sigma_j = E^E \delta \Delta \varepsilon_j^E \quad , \tag{28}$$

is column j of the material stiffness matrix. In practice, we simplified these operations as much as possible taking advantage at the structure of the material property matrices. This reduces the 12 x 12 problem to one 6 x 6 problem for the axial strains and three 2 x 2 problems for the shear strains. Furthermore, by taking advantage of material symmetry, the number of solutions was reduced to two 6 x 6 and two 2 x 2. The details are omitted for the sake of brevity.

5. Efficiency Comparison - Conclusions

The relative efficiency of different algorithms depends on a number of factors, such as the size of the problem, the constitutive law, the loading conditions, and the error tolerance. The example described here is not meant to give conclusions of general validity but rather to show how, in this particular case, an improved algorithm was needed to solve the problem.

The example described here is taken from the study of an irradiation specimen of relatively simple geometry. The finite element mesh, shown in Fig. 3, has 16 8-node elements and 71 nodes. The time history of nine time steps is one quarter of the complete irradiation history. In addition, this was a coupled thermomechanical analysis requiring about four iterations between the thermal and the stress analysis. Thus, the computer times described below should be multiplied by 16 to obtain the time for each case studied. Also, several analyses were performed of complete cross sections having six times the number of elements. By extrapolating the run times in the first two columns of Table 1, it was concluded that the initial strain method was not feasible for this study. Similar conclusions also apply to the full-sized fuel block (Fig. 1).

Table 1 shows a run time comparison for four different algorithms that were tried. The case in the first column, the initial strain method with one-step Runge Kutta, would have required around 200 time steps to remain below the stability limit. For these short steps, only two iterations per step were required. In the next column, initial strain with sub-steps, only nine time steps were needed for solution accuracy. However, with the initial strain method, about six iterations per step were needed to compensate for the inaccurate stiffness. The third column shows the first case with the consistent linearization method. The number of iterations is reduced by nearly a factor of four (note that the matrix is not updated in each time step). The cost, however, is only a factor of two better than the previous case because of the additional stress computations required to calculate the stiffness. Finally, the most favorable case was the consistent linearization with Crank-Nicholson integration. This reduced the cost of the element data processing by a factor of four. The total improvement ratio achieved in this sequence of changes is 889/58 = 15.3.

An additional improvement of about a factor of two can be realized for a linear viscoelastic material by calculating the stiffness looking ahead. By this method, iteration is avoided. However, since this procedure requires stiffness updates at every time step, it was not considered for permanent use in the TWOD code.

It is concluded that the consistent linearization method has been an effective algorithm for improving the efficiency of these viscoelastic calculations. Similar benefits are to be expected for nonlinear creep problems, particularly those now solved with the initial strain method. Continued study of this approach and a direct comparison with other algorithms in the literature appear to be warranted.

TABLE 1
COMPARISON OF FOUR SOLUTION ALGORITHMS

Stiffness Matrix	Elastic	Elastic	Consistent	Consistent
Integration Type	R-K	R-K	R-K	C-N
Integration Substeps?	No	Yes	Yes	No
Number of Time Steps	200	9	9	9
Number of Matrix Updates	5	5	5	5
Total Number of Iterations	400	69	21	19
Time of Matrix Factoring(s)	3.1	3.1	3.1	3.1
Time of Back Substitutions	60.	11.8	3.4	3.0
Time of Element Data Processing	800.	262.	96.2	25.9
Other Time	26.0	28.5	26.4	26.0
Total Running Time(s)	889.1	305.	129.	58.

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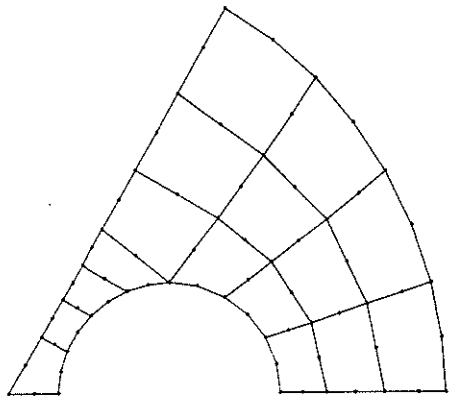

Figure 1. HTGR Fuel Elements

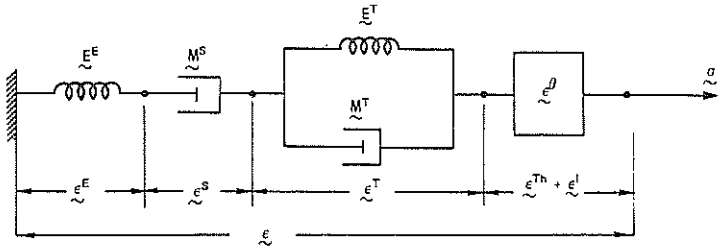

Figure 2. Maxwell-Kelvin Model of Graphite

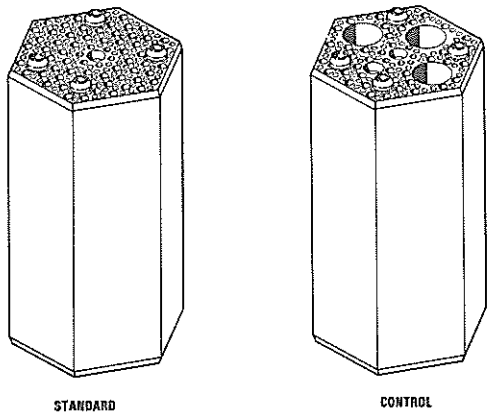

Figure 3. Irradiation Specimen, 60 Degree Sector