

Time Finite Element Discretization of Hamilton's Law of Varying Action

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Hamilton's Law of Varying Action is used as a variational source for the derivation of finite element discretization procedure in the time domain. Three different versions of the proposed algorithms are presented and verified for accuracy and stability. [The first one is the high-precision, finite time element, analogous to the standard finite elements, with cutoff frequency; the second version is the step by step, one-time element from which the unconditionally stable, with slightly altered accuracy, third algorithm is derived.] The new operator, connected with the proposed algorithms, bears attractive properties of much greater accuracy than other existing stable methods, and easy computer implementation. Thus, the work herein shows that the reservations expressed against the use of finite elements in time domain seem unjustified.

Nomenclature

a_T	= connectivity matrix
A, B, E, G	= global dynamic submatrices
c	= damping coefficient
C	= damping matrix
D	= global dynamic matrix
E	= global error vector
f	= load
F_i	= generalized path dependent forces
F, P	= global force vectors
H	= Hamilton function
$h^{\alpha\beta} H^{\alpha\beta}$	= local and global time coefficient matrices
k	= stiffness coefficient
K	= stiffness matrix
m	= mass
M	= mass matrix
q_i	= generalized coordinates
\dot{q}_i	= generalized velocities
q	= local displacement velocities vector
Q	= global displacement velocities vector
r	= truncation error vector
S	= variations
t	= time
t_0	= initial time
t_f	= final time
t_p	= period time
T	= kinetic energy
u	= displacement
\dot{u}	= velocity
V	= potential energy
Δt	= time increment
θ	= calculated frequency
μ	= calculated damping
ψ	= unknown constant
ω	= natural frequency
τ	= nondimensional time
ζ	= natural damping coefficient

I. Introduction

THIS paper is concerned²⁴ with the time domain solution by finite elements of discrete second-order linear equation systems of the form

$$M\ddot{u} + C\dot{u} + Ku = f \quad (1)$$

with the initial conditions:

$$u_{(t=0)} = u_0 \quad (2)$$

$$\dot{u}_{(t=0)} = \dot{u}_0 = v_0 \quad (3)$$

M , C , and K being the mass, damping, and stiffness matrices, and u and f the displacement and load vectors, respectively. Time derivatives are denoted by overdots.

The finite element method was originally developed for the approximate solution of boundary value problems. It was a natural step to attempt to develop similar methods for initial value problems. Some of these works have been summarized by Zienkiewicz¹ and Oden.² Strang and Fix³ have expressed serious reservations about the use of finite elements in the time domain. In their opinion, a straightforward application of the Galerkin principle may couple all of the time levels and destroy the crucial property of propagation forward in time. Indeed, almost all of the reported works which have applied a trial function/finite element discretization to the time domain deal with one finite domain of time and repeat the calculations for subsequent domains with new initial conditions. Simple linear,^{2,4,5} higher order Lagrange,^{1,6} and Hermitian cubic⁷⁻¹¹ interpolation functions for the displacement, or Hermitian interpolation functions for the inertia forces,^{12,13} were applied as trial functions within this time interval. The approximation was achieved, assuming that the full domain of investigation corresponds with that of this one time element, by Hamilton's principle,^{2,6-9} weighted residuals approach,¹ or directly with the equations of motion.^{10,12,13} Hence, all of these procedures lead to a step-by-step or recurrence calculation, unlike the common finite element procedures which produce simultaneous solutions of the whole range of interest. A standard finite element formulation in the time domain has been suggested in Refs. 14 and 15. Another attempt to formulate time finite elements based on Hamilton's law was made in Ref. 11 (see also Ref. 16).

The answer to the question of why the time dimension has not been treated equally with the spatial variables in the finite

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element discretization can be related, in part at least, to the development of variational methods, since much of the original stimulus in the development of finite element methods came from variational principles. While there are numerous variational principles for boundary value problems, few exist for initial value problems. In order of increasing generality, there are finite element methods based on: 1) extremum principles, 2) variational statements, and 3) the method of weighted residuals. The virtue of methods based on extremum principles is that one can develop numerical procedures that are guaranteed to be "well-behaved" in some sense. However, no extremum principles are known for initial-value problems, which rules out category 1. The advantage of the method of weighted residuals is that it can be applied to quite general equations, but it is not always clear how to choose the optimum weight factors. Variational statements may help in choosing suitable weighting functions. In a previous paper,¹⁷ the authors reintroduced such a variational statement characterizing the initial boundary value problem of mechanics (see also Ref. 18).

By applying the Ritz-Galerkin method, in which ordinary power series in the independent (time) variable was used, it was demonstrated¹⁷ how the different formulations of Hamilton's Law can be used to obtain approximate solutions of simple dynamic systems. The objective of this paper is to present the implementation of that new approach using finite elements in time.

Apart from avoiding the problems which can arise when higher powered polynomials are employed as basic functions,¹⁷ time finite element formulation has other advantages when used to solve problems in continuum mechanics, even though the principal motivation for the use of conventional finite elements has been the need to handle complicated boundary shapes (almost nonexistent in the time domain).³ Indeed, when the functions involved are sufficiently smooth, the number of time steps required to achieve acceptable accuracy may not be great and, in view of the increased storage required, the use of time finite elements to solve such a system is questionable. A version of the present algorithm applicable as a one-step method is given in the Appendix. There are many other cases, however, in which conventional step-by-step algorithms may call for a very large number of time steps. This is especially true when dealing with excitation and/or material properties changing rapidly in time. A physically based variational method, with its inherent stability¹⁹ and physical origin, may lower the computational effort considerably.

Thus, despite the reservations expressed by Strang and Fix,³ the extension of the finite element to the time domain is well motivated. A study that exploits the advantages afforded by the finite element discretization of time is given in Sec. III.

II. Time Finite Element

For the systems given in Eqs. (1-3) the general formulation of Hamilton's Law^{17,18,23,24} obtains the following form

$$A = \int_{t_0}^{t_f} (\dot{S}^T M \dot{q} - S^T C \dot{q} - S^T K q + S^T f) dt - S^T M \dot{q} \Big|_{t_0}^{t_f} = 0 \quad (4)$$

where $q(t)$ represents the displacement vector and $S(t)$ its variation. The usual symbol for variation of a function ($\delta q(t)$) was replaced here by a new function $S(t)$ in order to emphasize the mutual independence between the displacement and its variation.

Equation (4) can be discretized in time by subdividing the interval (t_0, t_f) into a number of time elements t_{j-1} to t_j . By prescribing a certain interpolation procedure for the time dependence, we may derive the values of q_i , \dot{q}_i and higher derivatives at any instant t , where $t_{j-1} \leq t \leq t_j$ in terms of their values at the instants t_{j-1} , t_j . In order to satisfy the equations

of motion, it is necessary to provide specifications for q_i and \dot{q}_i , since otherwise the initial dynamic conditions cannot be selected simply. Hence, the lowest order interpolation set is the third-order Hermitian interpolation polynomials. We will restrict ourselves here to these functions. Thus

$$q(t) = (1 - 3\tau^2 + 2\tau^3)q_{j-1} + (\tau - 2\tau^2 + \tau^3)\Delta t_j \dot{q}_{j-1} + (3\tau^2 - 2\tau^3)q_j + (-\tau^2 + \tau^3)\Delta t_j \dot{q}_j \quad (5)$$

and

$$\dot{q}(t)\Delta t_j = (-6\tau + 6\tau^2)q_{j-1} + (1 - 4\tau + 3\tau^2)\Delta t_j \dot{q}_{j-1} + (6\tau - 6\tau^2)q_j + (-2\tau + 3\tau^2)\Delta t_j \dot{q}_j \quad (6)$$

$\tau = t/\Delta t_j$ is a nondimensional time parameter ranging from 0 to 1. Similarly, for the load vector we obtain

$$f(t) = (1 - 3\tau^2 + 2\tau^3)f_{j-1} + (\tau - 2\tau^2 + \tau^3)\Delta t_j \dot{f}_{j-1} + (3\tau^2 - 2\tau^3)f_j + (-\tau^2 + \tau^3)\Delta t_j \dot{f}_j \quad (7)$$

We wish to ensure continuity of displacements and velocities between adjacent elements in the time domain and to impose two initial conditions for the solution of the second-order dynamic problem of Eqs. (1-3). It appears,^{22,24} however, that straightforward application of exactly the same approximation functions for the variables and for their variations, as is done in the standard "static" finite elements procedures, cause the time finite element to become unconditionally unstable. Equation (4) shows, however, possible separation between the actual approximate displacements q_i and the variations S_i ¹⁷ which, as emphasized before, are mutually independent. In other words, one can build q and S from different sets of functions. However, we will follow here the "physical path" for defining the variations of the state variables.¹⁷ The variations will be built up from the same set of admissible functions or their derivatives as the state variables. Suitable interpolation functions for the variations, built up from the same set of functions as for the displacement, appear to be the second derivatives of the cubic Hermitian functions. Thus

$$S(t) = (-6 + 12\tau)S_{j-1} + (-4 + 6\tau)\Delta t_j \dot{S}_{j-1} + (6 - 12\tau)S_j + (-2 + 6\tau)\Delta t_j \dot{S}_j \quad (8)$$

As shown later, the algorithms obtained by using the variations given in Eq. (8) are conditionally stable and highly efficient. In addition, the parent matrix obtained in this way is twice singular, which is in full agreement with the basic approach given in Ref. 17.

Substitutions for q , \dot{q} , f , and S from Eqs. (5-8) into Eq. (4) make it now possible to evaluate A of Eq. (4) in the typical j th time element. We thus find

$$A_j = \hat{S}_j^T [M \otimes h_j^{11} - C \otimes h_j^{01} - K \otimes h_j^{00}] \hat{q}_j + \hat{S}_j h_j^{00} \hat{f}_j \quad (9)$$

where

$$\begin{aligned} \hat{S}_j^T &= \{S_{j-1}^T; \Delta t_j \dot{S}_{j-1}^T; S_j^T; \Delta t_j \dot{S}_j^T\} \\ \hat{q}_j^T &= \{q_{j-1}^T; \Delta t_j \dot{q}_{j-1}^T; q_j^T; \Delta t_j \dot{q}_j^T\} \\ \hat{f}_j^T &= \{f_{j-1}^T; \Delta t_j \dot{f}_{j-1}^T; f_j^T; \Delta t_j \dot{f}_j^T\} \end{aligned} \quad (10)$$

h_j^{11} , h_j^{01} , h_j^{00} are given in the Appendix and \otimes stands for the outer product of matrices.

Assuming there are ℓ time elements and n degrees of freedom, we next form the $[n(2\ell+2) \times 1]$ vectors

$$\begin{aligned} Q^T &= \{q_0^T, \Delta t_0 \dot{q}_0^T, q_1^T, \Delta t_1 \dot{q}_1^T, \dots, q_j^T, \Delta t_j \dot{q}_j^T, \dots, q_\ell^T, \Delta t_\ell \dot{q}_\ell^T\} \\ S^T &= \{S_0^T, \Delta t_0 \dot{S}_0^T, S_1^T, \Delta t_1 \dot{S}_1^T, \dots, S_j^T, \Delta t_j \dot{S}_j^T, \dots, S_\ell^T, \Delta t_\ell \dot{S}_\ell^T\} \\ F^T &= \{f_0^T, \Delta t_0 \dot{f}_0^T, f_1^T, \Delta t_1 \dot{f}_1^T, \dots, f_j^T, \Delta t_j \dot{f}_j^T, \dots, f_\ell^T, \Delta t_\ell \dot{f}_\ell^T\} \end{aligned} \quad (11)$$

Assembly of the elemental expression (9) into a global system is performed via the global system of numbering relative to which the displacement vector Q and the load vector F are given.

The correlation between the elemental and global system is defined by

$$\hat{q}_j = a_{Tj} Q; \quad \hat{f}_j = a_{Tj} F \quad (12)$$

where a_{Tj} is the connectivity matrix of the j th element. The summation of the contributions A_j of all ℓ elements yields the following expression for A of Eq. (4)

$$A = S^T [M \otimes H^{11} - C \otimes H^{01} - K \otimes H^{00}] Q + S^T H^{00} F \quad (13)$$

where

$$H^{\alpha\beta} = a_T h^{\alpha\beta} a_T \quad (14)$$

with

$$\begin{aligned} h^{\alpha\beta} &= [h_1^{\alpha\beta} h_2^{\alpha\beta} \dots h_j^{\alpha\beta} \dots h_\ell^{\alpha\beta}] \\ a_T &= [a_{T1} a_{T2} \dots a_{Tj} \dots a_{T\ell}] \end{aligned} \quad (15)$$

As explained in Refs. 16 and 17, not all of the variations are arbitrary. This fact can be expressed in the following mathematical form

$$\frac{\partial A}{\partial S^T} = \psi \quad (16)$$

Six different consistent algorithms can now be obtained from Eq. (16). While any two from the following four variations $S_0, \dot{S}_0, S_\ell, \dot{S}_\ell$ are always imposed to be zero, the rest of the variations are arbitrary. However, the combination $\dot{S}_0 = \dot{S}_\ell = 0$ (formulation 3 of Ref. 17) is eliminated because of the particular structure of S in the present discussion. In accordance with Ref. 17, the two sets of equations which are multiplied by these two particular variations are equal to some undefined vector of constants. For example,

$$\psi^T = \{\psi_1^T, \psi_2^T, 0, 0, \dots, 0\}$$

when $S_0 = \dot{S}_0 = 0$ (formulation 1 of Ref. 17), or

$$\psi^T = \{\psi_1^T, 0, 0, \dots, 0, \dots, 0, \psi_2^T, 0\}$$

when $S_0 = S_\ell = 0$ (F2 of Ref. 17) etc. Hence, from Eq. (16)

$$[M \otimes H^{11} - C \otimes H^{01} - K \otimes H^{00}] Q + H^{00} F = \psi \quad (17)$$

or shortly

$$DQ = P + \psi \quad (18)$$

The set in Eq. (18) cannot be solved unless the initial values, for example, q_0, \dot{q}_0 of the specific problem, are introduced. In fact, they are imposed in Eq. (18) in the same manner as the boundary conditions are imposed in the standard finite element procedures. After the introduction of the initial values the two sets of equations which correspond to ψ_1 and ψ_2 can be eliminated. It follows that the restricted set of Eq.

(18) represents then $2n$ equations for the $2n$ unknowns $q_1, \dot{q}_1, \dots, q_\ell, \dot{q}_\ell$.

The five algorithms developed here are equivalent except at the "boundaries," i.e., only the first and the last two sets of equations are different. In fact, all of them can be rearranged to the form

$$\bar{D}\bar{Q} = \bar{P} + G_4 \begin{Bmatrix} q_0 \\ \dot{q}_0 \end{Bmatrix} \quad (19)$$

where

$$\begin{aligned} \bar{Q}^T &= [q_1^T, \dot{q}_1^T \Delta t, \dots, q_j^T, \dot{q}_j^T \Delta t, \dots, q_\ell^T, \dot{q}_\ell^T \Delta t] \\ \bar{P}^T &= [P_1^T, \dot{P}_1^T, \dots, P_j^T, \dot{P}_j^T, \dots, P_\ell^T, \dot{P}_\ell^T] \end{aligned} \quad (20)$$

and in the case of regular mesh Δt

$$\bar{D} = \begin{bmatrix} G_1 & & & G_2 & G_3 \\ B & E & & & \\ A & B & E & & \\ & A & B & E & \\ & & \dots & & \\ & & & & \dots \\ & & & & A & B & E \end{bmatrix} \quad (21)$$

and

$$\begin{aligned} A &= \begin{bmatrix} -M + \frac{\Delta t^2}{10} K & -\frac{1}{2} M + \frac{\Delta t}{12} C + \frac{\Delta t^2}{120} K \\ \frac{1}{2} M - \frac{\Delta t}{12} C - \frac{\Delta t^2}{120} K & \frac{1}{6} M - \frac{\Delta t}{24} C + \frac{\Delta t^2}{360} K \end{bmatrix} \\ B &= \begin{bmatrix} 2M - \frac{\Delta t^2}{5} K & -\frac{\Delta t}{6} C \\ \frac{\Delta t}{6} C & \frac{2}{3} M - \frac{\Delta t^2}{45} K \end{bmatrix} \\ E &= \begin{bmatrix} -M + \frac{\Delta t^2}{10} K & \frac{1}{2} M + \frac{\Delta t}{12} C - \frac{\Delta t^2}{120} K \\ -\frac{1}{2} M - \frac{\Delta t}{12} C + \frac{\Delta t^2}{120} K & \frac{1}{6} M + \frac{\Delta t}{24} C + \frac{\Delta t^2}{360} K \end{bmatrix} \end{aligned} \quad (22)$$

while,

$$\begin{aligned} P_j &= \frac{\Delta t^2}{120} (12f_{j-1} + \Delta t \dot{f}_{j-1} - 24f_j + 12f_{j+1} - \Delta t \dot{f}_{j+1}) \\ \dot{P}_j &= \frac{\Delta t^2}{360} (-3f_{j-1} + \Delta t \dot{f}_{j-1} - 8\Delta t \dot{f}_j + 3f_{j+1} + \Delta t \dot{f}_{j+1}) \end{aligned} \quad (23)$$

and G_1, G_2, G_3 , and G_4 are some known submatrices different for every formulation.

The most interesting algorithm, although not the best one, is the one which can be developed by assuming $S_j = \dot{S}_j = 0$ (formulation 4 of Ref. 17), for which $G_1 = E$ and $G_2 = G_3 = 0$. In this case, the matrix \bar{D} turns to be a pure low triangular matrix composed from three block diagonals. Hence, it enables us to obtain a special form of step-by-step solution procedure reproduced by the finite elements. This fact refutes

the reservation expressed against the use of finite elements in the time domain.

The step-by-step procedure obtained from formulation 4 of Ref. 17 is given by

$$\begin{aligned} E \begin{Bmatrix} q_1 \\ \dot{q}_1 \Delta t \end{Bmatrix} &= G_4 \begin{Bmatrix} q_0 \\ \dot{q}_0 \Delta t \end{Bmatrix} + \begin{Bmatrix} P_0 \\ \dot{P}_0 \end{Bmatrix} \\ E \begin{Bmatrix} q_j \\ \dot{q}_j \Delta t \end{Bmatrix} &= \begin{Bmatrix} P_{j-1} \\ \dot{P}_{j-1} \end{Bmatrix} - B \begin{Bmatrix} q_{j-1} \\ \dot{q}_{j-1} \Delta t \end{Bmatrix} - A \begin{Bmatrix} q_{j-2} \\ \dot{q}_{j-2} \Delta t \end{Bmatrix} \quad j=2, \dots, \ell \end{aligned} \quad (24)$$

Note that the starting values q_0 , \dot{q}_0 can be imposed in a natural way. The remaining four algorithms cannot be expressed in the same manner. However, they are very similar and possess almost the same computational characteristics, i.e., accuracy and stability, as the one discussed.

III. Verification of the Algorithm

The damping matrix is usually assumed to be proportional either to the mass or to the stiffness matrix or, in parts, to both of them. Exploiting the orthogonality of the modal matrix of the system, Eq. (1) may be decomposed into a set of single equations of the form:

$$m\ddot{u} + c\dot{u} + ku = f \quad (25)$$

Hence, all the analysis of the algorithms will be made by investigation of a single degree of freedom. It must be emphasized, however, that the algorithms in the general case do not require the system to be decomposed or even to possess natural modes. Assuming regular mesh Δt , a typical row (or rather pairs of rows, since there are two unknowns, q_j and \dot{q}_j , at the mesh point $t_j = j\Delta t$) of the system Eq. (19) is

$$\begin{aligned} &\left(-m + \frac{\Delta t^2}{10}k\right)q_{j-1} + \left(-\frac{1}{2}m + \frac{\Delta t}{12}c + \frac{\Delta t^2}{120}k\right)\Delta t \dot{q}_{j-1} \\ &+ \left(2m - \frac{\Delta t^2}{5}k\right)q_j - \frac{\Delta t^2}{6}c\dot{q}_j + \left(-m + \frac{\Delta t^2}{10}k\right)q_{j+1} \\ &+ \left(\frac{1}{2}m + \frac{\Delta t}{12}c - \frac{\Delta t^2}{120}k\right)\Delta t \dot{q}_{j+1} \\ &= -\frac{\Delta t^2}{120}(12f_{j-1} + \Delta t \dot{f}_{j-1} - 24f_j + 12f_{j+1} - \Delta t \dot{f}_{j+1}) \end{aligned} \quad (26)$$

$$\begin{aligned} &\left(\frac{1}{2}m - \frac{\Delta t}{12}c - \frac{\Delta t^2}{120}k\right)q_{j-1} + \left(\frac{1}{6}m - \frac{\Delta t}{24}c + \frac{\Delta t^2}{360}k\right)\Delta t \dot{q}_{j-1} \\ &+ \frac{\Delta t}{6}c\dot{q}_j + \left(\frac{2}{3}m - \frac{\Delta t^2}{45}k\right)\Delta t \dot{q}_j + \left(-\frac{1}{2}m - \frac{\Delta t}{12}c\right. \\ &+ \left.\frac{\Delta t^2}{120}k\right)q_{j+1} + \left(\frac{1}{6}m + \frac{\Delta t}{24}c + \frac{\Delta t^2}{360}k\right)\Delta t \dot{q}_{j+1} \\ &= -\frac{\Delta t^2}{360}(-3f_{j-1} + \Delta t \dot{f}_{j-1} - 8\Delta t \dot{f}_j + 3f_{j+1} + \Delta t \dot{f}_{j+1}) \end{aligned} \quad (27)$$

One can see that instead of operating with the unknown q_j only where there is always one equation per mesh point, the finite element difference equation couples both displacement and velocities as unknowns. However, the equation for the velocity is formally consistent with the original equation differentiated once. The result is that high accuracy can be achieved without abandoning the strictly local nature of the difference equation.

Consistency

The local truncation error of the difference equations (26) and (27) is calculated by applying the discrete algorithm to the values of the true solution expanded into Taylor series. The following conditions are assumed to hold throughout this section: 1) in Eqs. (26) and (27), f is an interpolate of the exact load distribution; 2) possible jumps in the fifth and lower derivatives of the true loading function are located at the elemental boundaries. In other words, the sixth derivative of the loading function is finite along every elemental domain. Let the values of the exact distribution be distinguished from the approximated entities by addition of an asterisk. Accordingly, q^* will be the exact solution of Eqs. (1-3) for the loading f^* . Let us start with the assumptions

$$\begin{aligned} q_j^* &= q(j\Delta t) + e(j\Delta t) & \dot{q}_j^* &= \dot{q}(j\Delta t) + \epsilon(j\Delta t) \\ f_j^* &= f(j\Delta t) & \dot{f}_j^* &= \dot{f}_j(j\Delta t) \end{aligned} \quad (28)$$

and expand $q_{j\pm 1}^*$, $\dot{q}_{j\pm 1}^*$, $f_{j\pm 1}^*$, $\dot{f}_{j\pm 1}^*$ about the central point $(j\Delta t)$. The truncation error of the algorithm is now obtained by replacing the approximate values by the true ones in Eqs. (26) and (27).

Equations (26) and (27) yield

$$\begin{aligned} R_q &= -\frac{\Delta t^4}{12} \left[m\ddot{q}^{(4)*} + c\dot{q}^{(3)*} + k\ddot{q}^{(2)*} - f^{(2)*} + \frac{\Delta t^2}{15} (m\ddot{q}^{(6)*} \right. \\ &\quad \left. + c\dot{q}^{(5)*} + k\ddot{q}^{(4)*} - f^{(4)*}) + \frac{\Delta t^4}{600} (m\ddot{q}^{(8)*} + c\dot{q}^{(7)*} + k\ddot{q}^{(6)*} - f^{(6)*}) \right. \\ &\quad \left. + \frac{\Delta t^2}{60} c\dot{q}^{(5)*} + \frac{\Delta t^4}{8400} m\ddot{q}^{(8)*} + \frac{\Delta t^4}{900} c\dot{q}^{(7)*} + O(\Delta t^6) \right] \\ &\cong -\frac{\Delta t^6}{720} c\dot{q}^{(5)*} + \frac{\Delta t^8}{100800} m\ddot{q}^{(8)*} + \frac{\Delta t^8}{10800} c\dot{q}^{(7)*} \end{aligned} \quad (29)$$

$$\begin{aligned} R_{\dot{q}\Delta t} &= -\frac{\Delta t^5}{180} \left[m\ddot{q}^{(5)*} + c\dot{q}^{(4)*} + k\ddot{q}^{(3)*} - f^{(3)*} \right. \\ &\quad \left. + \frac{\Delta t^2}{15} (m\ddot{q}^{(7)*} + c\dot{q}^{(6)*} + k\ddot{q}^{(5)*} - f^{(5)*}) + \frac{1}{4} c\dot{q}^{(4)*} \right. \\ &\quad \left. - \frac{2\Delta t^2}{105} m\ddot{q}^{(7)*} + \frac{\Delta t^2}{60} c\dot{q}^{(6)*} + O(\Delta t^4) \right] \cong -\frac{\Delta t^6}{720} c\dot{q}^{(4)*} \\ &\quad - \frac{\Delta t^8}{9450} m\ddot{q}^{(7)*} + \frac{\Delta t^8}{10800} c\dot{q}^{(6)*} \end{aligned} \quad (30)$$

Accordingly, the complete truncation error vector takes the form:

$$r = \begin{Bmatrix} R_q \\ R_{\dot{q}\Delta t} \end{Bmatrix} = \frac{c\Delta t^6}{720} \begin{Bmatrix} \ddot{q}^{(5)*} + \frac{\Delta t^2}{15} \ddot{q}^{(7)*} \\ \dot{q}^{(4)*} + \frac{\Delta t^2}{15} \dot{q}^{(6)*} \end{Bmatrix} + \frac{m\Delta t^8}{9450} \begin{Bmatrix} \frac{32}{3} \ddot{q}^{(8)*} \\ -\dot{q}^{(7)*} \end{Bmatrix} \quad (31)$$

It is worth mentioning that the displacement and velocity local truncation errors are of the same order and in the absence of damping, the local truncation error is of order 8.

Convergence

We define the error E as

$$E = \bar{Q}^* - \bar{Q} \quad (32)$$

The relation for the error is obtained by subtracting Eq. (19) from

$$\bar{D}\bar{Q}^* = \bar{P}^* + G_4 \left\{ \frac{q_0^*}{q_0^* \Delta t} \right\} + R \quad (33)$$

where R is the general truncation error vector obtained from Eq. (31). Remembering that $P^* = P$, $q_0^* = q_0$, $\dot{q}_0^* = \dot{q}_0$ and multiplying the result by \bar{D}^{-1} yields

$$E = \bar{D}^{-1} R \quad (34)$$

Hence

$$\|E\|_\infty \leq \|\bar{D}^{-1}\|_\infty \|R\|_\infty \quad (35)$$

Recognizing from Eqs. (21) and (22) particularly for the F4 algorithm (formulation 4 of Ref. 17) that $\|\bar{D}^{-1}\| \leq \mu/\Delta t^2$ where μ is some finite constant function of m , k , and c , we arrive at the convergence estimate,

$$\begin{aligned} \|E\|_\infty &\leq \mu_1 (\Delta t)^4; \text{ with damping} \\ \|E\|_\infty &\leq \mu_2 (\Delta t)^6; \text{ without damping} \end{aligned} \quad (36)$$

Stability

Better perception of the stability and accuracy characteristic may be obtained by the frequency method which makes systematic use of the Fourier series.³ The pair of finite difference equations, Eqs. (26) and (27), are solved in the homogeneous case by

$$q_j = c_1 z^j \quad \dot{q}^j = c_2 z^j \quad (37)$$

where c_1 and c_2 are determined by the initial conditions. Substitution of q_j and \dot{q}_j in Eqs. (26) and (27) and elimination of the constants between them yields the characteristic equation

$$\begin{aligned} z^4 - \frac{4m^2 + \Delta t m c - \frac{11}{15} \Delta t^2 k m + \frac{1}{3} \Delta t^2 c^2 + \frac{1}{15} \Delta t^3 k c + \frac{1}{30} \Delta t^4 k^2}{m^2 + \frac{1}{2} \Delta t m c + \frac{1}{15} \Delta t^2 k m + \frac{1}{12} \Delta t^2 c^2 + \frac{1}{30} \Delta t^3 k c + \frac{1}{240} \Delta t^4 k^2} z^3 + \frac{6m^2 - \frac{8}{5} \Delta t^2 k m + \frac{1}{2} \Delta t^2 c^2 + \frac{7}{120} \Delta t^4 k^2}{m^2 + \frac{1}{2} \Delta t m c + \frac{1}{15} \Delta t^2 k m + \frac{1}{12} \Delta t^2 c^2 + \frac{1}{30} \Delta t^3 k c + \frac{1}{240} \Delta t^4 k^2} z^2 \\ - \frac{4m^2 - \Delta t m c - \frac{11}{15} \Delta t^2 k m + \frac{1}{3} \Delta t^2 c^2 - \frac{1}{15} \Delta t^3 k c + \frac{1}{30} \Delta t^4 k^2}{m^2 + \frac{1}{2} \Delta t m c + \frac{1}{15} \Delta t^2 k m + \frac{1}{12} \Delta t^2 c^2 + \frac{1}{30} \Delta t^3 k c + \frac{1}{240} \Delta t^4 k^2} z + \frac{m^2 - \frac{1}{2} \Delta t m c + \frac{1}{15} \Delta t^2 k m + \frac{1}{12} \Delta t^2 c^2 - \frac{1}{30} \Delta t^3 k c + \frac{1}{240} \Delta t^4 k^2}{m^2 + \frac{1}{2} \Delta t m c + \frac{1}{15} \Delta t^2 k m + \frac{1}{12} \Delta t^2 c^2 + \frac{1}{30} \Delta t^3 k c + \frac{1}{240} \Delta t^4 k^2} = 0 \end{aligned} \quad (38)$$

Equation (38) is solved by the double root $z = 1$ (stands for the initial conditions) and then reduces to the quadratic

$$z^2 - 2 \frac{m^2 - \frac{13}{30} \Delta t^2 k m + \frac{1}{12} \Delta t^2 c^2 + \frac{1}{80} \Delta t^4 k^2}{m^2 + \frac{1}{2} \Delta t m c + \frac{1}{15} \Delta t^2 k m + \frac{1}{12} \Delta t^2 c^2 + \frac{1}{30} \Delta t^3 k c + \frac{1}{240} \Delta t^4 k^2} z + \frac{m^2 - \frac{1}{2} \Delta t m c + \frac{1}{15} \Delta t^2 k m + \frac{1}{12} \Delta t^2 c^2 - \frac{1}{30} \Delta t^3 k c + \frac{1}{240} \Delta t^4 k^2}{m^2 + \frac{1}{2} \Delta t m c + \frac{1}{15} \Delta t^2 k m + \frac{1}{12} \Delta t^2 c^2 + \frac{1}{30} \Delta t^3 k c + \frac{1}{240} \Delta t^4 k^2} = 0 \quad (39)$$

from which the two principal roots are obtained. Assuming $m \neq 0$ we shall make use of the following relation

$$\omega^2 = k/m \quad \zeta = c/2m \quad (40)$$

to write the roots as

$$z = \frac{\left[1 - \frac{13}{30} (\omega \Delta t)^2 + \frac{1}{80} (\omega \Delta t)^4 + \frac{1}{3} (\zeta \Delta t)^2 \right] \pm \left\{ (\zeta \Delta t)^2 \left[1 - \frac{(\omega \Delta t)^2}{10} \right]^2 - (\omega \Delta t)^2 \left[1 - \frac{(\omega \Delta t)^2}{10} \right] \left[1 - \frac{(\omega \Delta t)^2}{10} + \frac{(\omega \Delta t)^4}{720} \right] \right\}^{1/2}}{1 + \frac{1}{15} (\omega \Delta t)^2 + \frac{1}{240} (\omega \Delta t)^4 + (\zeta \Delta t) + \frac{1}{3} (\zeta \Delta t)^2 + \frac{1}{15} (\zeta \Delta t) (\omega \Delta t)^2} \quad (41)$$

In the absence of damping, the roots are complex conjugate with modulus equal to unity, provided $(\omega\Delta t)^2 < 10$ which corresponds to $\Delta t/T_p < 0.503$ where T_p is the period of the oscillator. A version of the present algorithm which has infinite cutoff frequency is given in the Appendix. Thus, in the absence of damping, up to the cutoff frequency the solution is purely oscillatory with no artificial damping and the frequency is presented by

$$tg(\theta\Delta t) = \frac{(\omega\Delta t) \left(1 - \frac{(\omega\Delta t)^2}{10} + \frac{(\omega\Delta t)^4}{720}\right)^{1/2} \left(1 - \frac{(\omega\Delta t)^2}{10}\right)^{1/2}}{\left(1 - \frac{13(\omega\Delta t)^2}{30} + \frac{(\omega\Delta t)^4}{80}\right)} \quad (42)$$

For small $(\omega\Delta t)$

$$(\theta\Delta t) = (\omega\Delta t) \left[1 - \frac{1}{1440} (\omega\Delta t)^4\right] \quad (43)$$

implying that the error in the frequency with the scheme is $O(\omega\Delta t)^4$. It is worth mentioning that the general two-step algorithms developed by finite difference procedures (Newmark's β family) are, at most, of third order as linear acceleration method or of second order as the central difference scheme or the unconditionally stable average acceleration method.²⁰ The same holds for the algorithms developed through weighted residuals methods.¹

In the presence of damping, up to the cutoff frequency the roots are less than one, and for

$$\zeta < \omega \left[\frac{1 - \frac{(\omega\Delta t)^2}{10} + \frac{(\omega\Delta t)^4}{720}}{1 - \frac{(\omega\Delta t)^2}{10}} \right]^{1/2} \quad (44)$$

they are complex while for

$$\zeta \geq \omega \left[\frac{1 - \frac{(\omega\Delta t)^2}{10} + \frac{(\omega\Delta t)^4}{720}}{1 - \frac{(\omega\Delta t)^2}{10}} \right]^{1/2} \quad (45)$$

they become real. The approximate solution, therefore, copies almost perfectly the oscillating or decaying behavior of the true solution. The damping is given by

$$e^{-\mu\Delta t} = \frac{1 + \frac{1}{15}(\omega\Delta t)^2 + \frac{1}{240}(\omega\Delta t)^4 + \frac{1}{3}(\zeta\Delta t)^2 - (\zeta\Delta t) \left[1 + \frac{1}{15}(\omega\Delta t)^2\right]}{1 + \frac{1}{15}(\omega\Delta t)^2 + \frac{1}{240}(\omega\Delta t)^4 + \frac{1}{3}(\zeta\Delta t)^2 + (\zeta\Delta t) \left[1 + \frac{1}{15}(\omega\Delta t)^2\right]} \quad (46)$$

and the damping error may be assessed from the ratio $e^{-\mu\Delta t}/e^{-\zeta\Delta t}$. For small $(\zeta\Delta t)$ and $(\omega\Delta t)$ this may be written approximately as

$$e^{-\mu\Delta t} = e^{-\zeta\Delta t} \left[1 - \frac{2}{45}(\omega\Delta t)^2(\zeta\Delta t)\right] \quad (47)$$

so that increasing Δt reduces the effective damping, while the effective dynamic frequency is represented by

$$tg(\bar{\theta}\Delta t) = \frac{\left\{(\omega\Delta t)^2 \left[1 - \frac{(\omega\Delta t)^2}{10}\right] \left[1 - \frac{(\omega\Delta t)^2}{10} + \frac{(\omega\Delta t)^4}{720}\right] - (\zeta\Delta t)^2 \left[1 - \frac{(\omega\Delta t)^2}{10}\right]^2\right\}^{1/2}}{1 - \frac{13(\omega\Delta t)^2}{30} + \frac{(\omega\Delta t)^4}{80} + \frac{(\zeta\Delta t)^2}{3}} \quad (48)$$

and the frequency error is given by $(\bar{\theta}\Delta t/\omega\Delta t) - 1$, where the dynamic frequency is defined by

$$\bar{\omega}^2 = \omega^2 - \zeta^2$$

For small $(\omega\Delta t)$ and $(\zeta\Delta t)$ the dynamic frequency error is given by

$$(\bar{\theta}\Delta t) = (\omega\Delta t) [1 - O((\omega\Delta t)^4)] \quad (49)$$

IV. Numerical Examples

The method discussed in the preceding paragraphs is now applied to two simple examples and the accuracy of the results is compared with the exact ones. The first example is the free motion due to a unit initial displacement of a one-degree-of-freedom damped harmonic oscillator. Presuming consistent physical dimensions the following numerical values are taken: $m=1$ and $k=4\pi^2$. Some trivial calculations yield the values of the natural frequency ω , the associated period t_p , and the critical damping as

$$\omega = (k/m)^{1/2} = 2\pi, \quad t_p = 2\pi/\omega = 1, \quad \zeta_{crit} = 2\pi$$

Three cases are considered: 1) $\zeta=0$; 2) $\zeta=\pi/4$; and 3) $\zeta=8\pi$. The calculated displacement and velocity at various times for systematically refined time elements are compared with the exact values in Tables 1-3. Figures 1-3 show the convergence plots. As is easily recognized, the computed slopes are very close to the theoretical values.

As an illustration of application of the algorithm to multidegree of freedom systems, the second example is a forced motion of a two-degree-of-freedom harmonic oscillator governed by a resonant load. (See Fig. 4.) Again presuming consistent physical dimensions, the numerical values taken are

$$m_1=4, \quad m_2=2, \quad k_1=2, \quad k_2=1$$

yielding

$$\omega_1 = 1/4, \quad \omega_2 = 1 \quad \text{and} \quad t_{p1} = 8\pi, \quad t_{p2} = 2\pi$$

and

$$u_1(0) = u_2(0) = \dot{u}_1(0) = \dot{u}_2(0) = f_1 = 0; \quad f_2 = \sin t$$

Computed results compared with the exact values along an interval of $6t_{p2}$ are shown in Fig. 4. Very good agreement with

Table 3 $\zeta = 8\pi$

$\Delta t/t_p$	T/t_p	u	\dot{u}
1/2	1	0.1940556	-0.1969754
1/4	1	0.2000000	-0.1949172
1/8	1	0.2000708	-0.1945524
1/16	1	0.2000735	-0.1944712
Exact	1	0.2000736	-0.2944740
1/2	20	-9.801337×10^{-5}	$-0.1414201 \times 10^{-5}$
1/4	20	0.127851×10^{-4}	$-0.1571334 \times 10^{-7}$
1/16	20	1.242945×10^{-8}	$-0.1473126 \times 10^{-8}$
Exact	20	0.256475×10^{-4}	$-0.2492800 \times 10^{-14}$

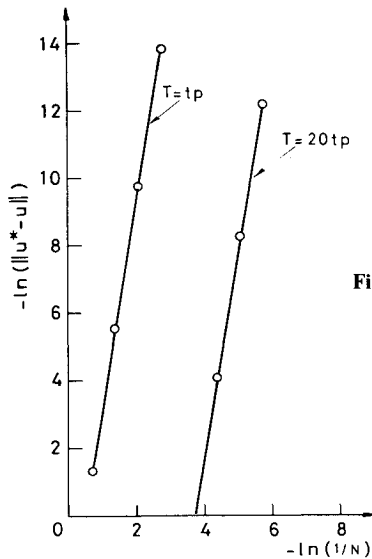
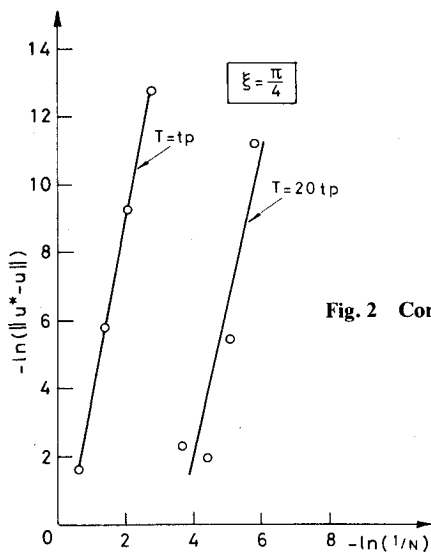
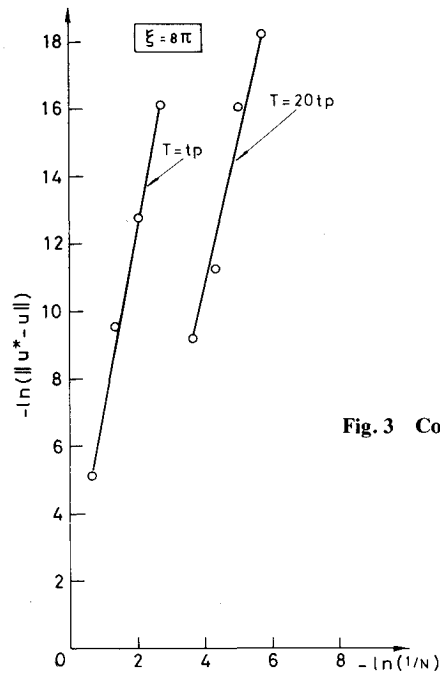
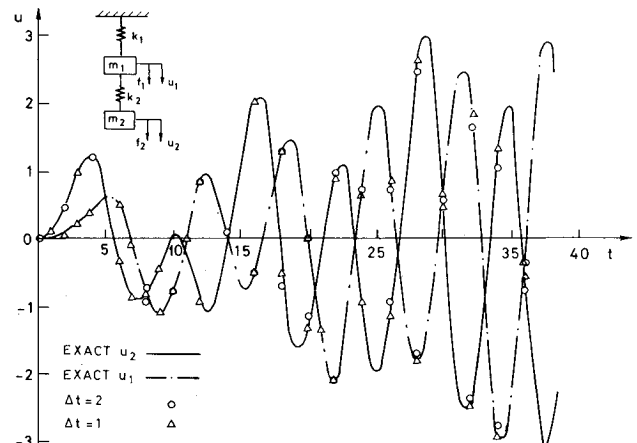
Fig. 1 Convergence plot, $\zeta = 0$.Fig. 2 Convergence plot, $\zeta = \pi/4$.Fig. 3 Convergence plot, $\zeta = 8\pi$.

Fig. 4 Two-degrees-of-freedom harmonic oscillator in resonance.

the true solution is achieved with t_{p2}/π mesh already giving results of four-decimal accuracy.

V. Discussion and Conclusions

The finite element method based on the variational statement of Hamilton's Law and applied in the time domain has been found capable of systematic derivation of many new extensively highly accurate procedures for the solution of initial value problems. Thus, the reservation expressed against the use of finite elements in the time dimension has been found unjustified. Here a scheme is derived in which velocities and displacements are simultaneously interpolated by a "conforming" cubic function. The variations functions are derived from the same functions. Obviously, many other

alternatives of using higher trial functions or different variations functions within the variational statement are possible. With six different variational formulations, the possibilities are clearly infinite.

Three different versions of the proposed algorithms have been presented. The first one is the high-precision, finite time elements (analogous to the standard finite elements) with cutoff frequency; the second version is the step-by-step, one time element, from which the unconditionally stable, with slightly altered accuracy, third technique has been derived. The choice between them cannot be decided independently of the problem in hand, the programming techniques, and type of computer available. In general, when the response affects only the lower frequencies, the unconditionally stable, step-by-step version with large elements will be most economical. For problems in which the higher modes enter with their own frequencies, the high-precision time elements version becomes more efficient. This is particularly true of impulse and wave problems. The presented algorithms may be modified further to have some artificial damping, but it seems better to use them in the form presented here. Artificial damping must be avoided completely when using these methods to investigate problems sensitive to small amounts of damping. Aeroelastic

excitation is an obvious case in point. Although the present paper is limited to constant coefficient linear cases, the proposed methods are capable of handling problems with time-dependent coefficients, both damping and stiffness positive, as well as negative and nonlinear problems. These questions are the subject of investigations presently being made.

Appendix

Matrices of the Temporal Element

The matrices for the temporal element of Eq. (9) are as follows:

$$[h^{II}] = \frac{12}{\Delta t} \begin{bmatrix} 1 & \frac{1}{2} & -1 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{3} & -\frac{1}{2} & \frac{1}{6} \\ -1 & -\frac{1}{2} & 1 & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{6} & -\frac{1}{2} & \frac{1}{3} \end{bmatrix}, [h^{0I}] = -\frac{1}{2} \begin{bmatrix} 0 & -2 & 0 & 2 \\ 2 & -1 & -2 & 1 \\ 0 & 2 & 0 & -2 \\ -2 & -1 & 2 & 1 \end{bmatrix}, [h^{00}] = -\frac{m\Delta t}{30} \begin{bmatrix} -36 & -3 & 36 & -3 \\ -33 & -4 & 3 & 1 \\ 36 & 3 & -36 & 3 \\ -3 & 1 & 33 & -4 \end{bmatrix} \quad (A1)$$

One Time Element—Step-by-Step Algorithm

Assuming that the full domain of investigation corresponds with that of one element, by inserting Eqs. (10) and (A1), Eq. (9) can now be written for a one-degree-of-freedom system as

$$A = \begin{bmatrix} S_0 \\ \dot{S}_0 \Delta t \\ S_1 \\ \dot{S}_1 \Delta t \end{bmatrix}^T \begin{bmatrix} m - \frac{\Delta t^2}{10} k & \frac{1}{2} m - \frac{\Delta t}{12} c - \frac{\Delta t^2}{120} k & -m + \frac{\Delta t^2}{10} k & \frac{1}{2} m + \frac{\Delta t}{12} c - \frac{\Delta t^2}{120} k \\ \frac{1}{2} m + \frac{\Delta t}{12} c - \frac{11\Delta t^2}{120} k & \frac{1}{3} m - \frac{\Delta t}{24} c - \frac{\Delta t^2}{90} k & -\frac{1}{2} m - \frac{\Delta t}{12} c + \frac{\Delta t^2}{120} k & \frac{1}{6} m + \frac{\Delta t}{24} c + \frac{\Delta t^2}{360} k \\ -m + \frac{\Delta t^2}{10} k & -\frac{1}{2} m + \frac{\Delta t}{12} c + \frac{\Delta t^2}{120} k & m - \frac{\Delta t^2}{10} k & -\frac{1}{2} m - \frac{\Delta t}{12} c + \frac{\Delta t^2}{120} k \\ \frac{1}{2} m - \frac{\Delta t}{12} c - \frac{\Delta t^2}{120} k & \frac{1}{6} m - \frac{\Delta t}{24} c + \frac{\Delta t^2}{360} k & -\frac{1}{2} m - \frac{\Delta t}{12} c + \frac{11\Delta t^2}{120} k & \frac{1}{3} m + \frac{\Delta t}{24} c - \frac{\Delta t^2}{90} k \end{bmatrix} \begin{bmatrix} q_0 \\ \dot{q}_0 \Delta t \\ q_1 \\ \dot{q}_1 \Delta t \end{bmatrix} \\ + \begin{bmatrix} S_0 \\ \dot{S}_0 \Delta t \\ S_1 \\ \dot{S}_1 \Delta t \end{bmatrix}^T \frac{\Delta t^2}{360} \begin{bmatrix} 36 & 3 & -36 & 3 \\ 33 & 4 & -3 & -1 \\ -36 & -3 & 36 & -3 \\ 3 & -1 & -33 & 4 \end{bmatrix} \begin{bmatrix} f_0 \\ \dot{f}_0 \Delta t \\ f_1 \\ \dot{f}_1 \Delta t \end{bmatrix} \quad (A2)$$

We may now apply the conditions of Eq. (2) in one of the five forms described in Sec. II. Remarkably, it turns out here that after applying Eq. (16), inserting the initial conditions, and eliminating the two equations which correspond to ψ_1 and ψ_2 , all five described forms yield completely to equivalent sets of two equations for the two unknowns q_1 and \dot{q}_1 in the form

$$D_1 \begin{Bmatrix} q_1 \\ \dot{q}_1 \Delta t \end{Bmatrix} = D_0 \begin{Bmatrix} q_0 \\ \dot{q}_0 \Delta t \end{Bmatrix} + D_f \begin{Bmatrix} f_0 \\ \dot{f}_0 \Delta t \\ f_1 \\ \dot{f}_1 \Delta t \end{Bmatrix} \quad (A3)$$

where

$$[D_1] = \begin{bmatrix} -\frac{1}{2} m - \frac{\Delta t}{12} c + \frac{\Delta t^2}{120} k & \frac{1}{6} m + \frac{\Delta t}{24} c + \frac{\Delta t^2}{360} k \\ -\frac{1}{2} m + \frac{\Delta t}{12} c + \frac{11\Delta t^2}{120} k & \frac{1}{3} m + \frac{\Delta t}{12} c - \frac{\Delta t^2}{90} k \end{bmatrix} \quad [D_0] = \begin{bmatrix} -\frac{1}{2} m - \frac{\Delta t}{12} c + \frac{11\Delta t^2}{120} k & -\frac{1}{3} m + \frac{\Delta t}{24} c + \frac{\Delta t^2}{90} k \\ -\frac{1}{2} m + \frac{\Delta t}{12} c + \frac{\Delta t^2}{120} k & -\frac{1}{6} m + \frac{\Delta t}{24} c - \frac{\Delta t^2}{360} k \end{bmatrix} \\ [D_f] = \frac{\Delta t^2}{360} \begin{bmatrix} -33 & -4 & 3 & 1 \\ -3 & 1 & 33 & -4 \end{bmatrix} \quad (A4)$$

Since every finite element is an autonomous time interval, the initial conditions can be imposed at every time node leading to a step-by-step algorithm. Hence, the stability and accuracy analysis can be made by investigation of the amplification matrix $AM = D_1^{-1} D_0$. Trivial calculations reveal that the algorithm is stable up to $(\omega \Delta t)^2 \leq 10$ and of order four.

In the next section, it will be shown that a modification can be brought to the presented algorithm to make it unconditionally stable without significant alteration in its accuracy properties.

The Modified Algorithm with Unconditional Stability

Bathe and Wilson²¹ have described a procedure to modify the stability properties of Newmark's linear acceleration method. The idea used was to assume a linear variation of acceleration over a time interval $\Delta t' = \theta \Delta t$ larger than the step size Δt ($\theta = 1$), and then calculate velocities and displacement at the earlier time instant t_{n+1} from interpolations formulas.

The path followed here to extend the stability range of the one time element step-by-step algorithm is very similar. The response is first calculated at the later time $t_{n+\alpha \Delta t}$:

$$D'_1 \begin{Bmatrix} q_{n+\alpha} \\ \dot{q}_{n+\alpha} \Delta t \end{Bmatrix} = D'_0 \begin{Bmatrix} q_n \\ \dot{q}_n \Delta t \end{Bmatrix} + D'_f \begin{Bmatrix} f_n \\ \dot{f}_n \Delta t \\ f_{n+\alpha} \\ \dot{f}_{n+\alpha} \Delta t \end{Bmatrix} \quad (A5)$$

with

$$D'_0 = D_0(\alpha \Delta t); \quad D'_1 = D_1(\alpha \Delta t) \quad \text{and} \quad D'_f = D_f(\alpha \Delta t) \quad (A6)$$

Using then the interpolation formulas (5) and (6) to calculate the displacement and velocities at time t_{n+1} yields

$$\begin{Bmatrix} q_{n+1} \\ \dot{q}_{n+1} \Delta t \end{Bmatrix} = AT_1^{-1} \begin{Bmatrix} q_{n+\alpha} \\ \dot{q}_{n+\alpha} \Delta t \end{Bmatrix} - AT_1^{-1} AT_0 \begin{Bmatrix} q_n \\ \dot{q}_n \Delta t \end{Bmatrix} \quad (A7)$$

with the definition

$$AT_0(\alpha) = \begin{bmatrix} (1-\alpha)^2(1+2\alpha) & \alpha(1-\alpha)^2 \\ 6\alpha(\alpha-1) & (1+\alpha)(1-3\alpha) \end{bmatrix}$$

$$AT_1(\alpha) = \begin{bmatrix} (3-2\alpha)\alpha^2 & \alpha^2(\alpha-1) \\ 6\alpha(1-\alpha) & \alpha(3\alpha-2) \end{bmatrix} \quad (A8)$$

It turns out that the integration scheme defined by Eqs. (A5) and (A7) becomes unconditionally stable when $\alpha \geq 1.06$, and that no significant change in the accuracy is observed for α close to that value.

The consistent algorithm defined by Eqs. (A5) and (A7) thus bears attractive properties: unconditional stability and much greater accuracy than other existing unconditionally stable schemes.

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