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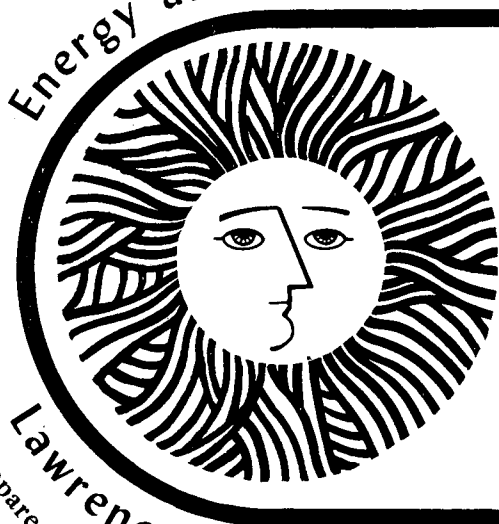
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Collocation, Dissipation And "Overshoot"
For Time Integration Schemes In
Structural Dynamics

Hans M. Hilber and Thomas J.R. Hughes

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COLLOCATION, DISSIPATION AND "OVERSHOOT" FOR TIME INTEGRATION SCHEMES
IN STRUCTURAL DYNAMICS

by

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ABSTRACT

The concept of collocation, originally used by Wilson in the development of dissipative algorithms for structural dynamics, is systematically generalized and analyzed. Optimal schemes within this class are developed and compared with a recently proposed family of dissipative algorithms, called α methods. The α methods are found to be superior on the basis of standard measures of dissipation and dispersion.

It is pointed out that the tendency to overshoot is an important and independent factor which should be considered in an evaluation of an implicit scheme. The basis for studying overshoot is discussed and the optimal collocation and α methods are compared. It is found that pathological overshooting is an inherent property of collocation schemes, whereas the overshooting characteristics of the α methods are good.

1. INTRODUCTION

Considerable effort has gone into the development of efficient computational methods for the step-by-step integration of the equations of structural dynamics (see for example [1-4, 7-20, 22]). Although there is no universal consensus, it is generally agreed that for a method to be competitive it should possess the following attributes:

1. Unconditional stability when applied to linear problems.
2. No more than one set of implicit equations should have to be solved at each step.
3. Second-order accuracy.
4. Controllable algorithmic dissipation in the higher modes.
5. Self-starting.

Conditionally stable algorithms require that a time step be taken which is less than a constant times the smallest period of the structure. In complicated structural models, containing slender members exhibiting bending effects, this restriction is a stringent one and often entails using time steps which are much smaller than those

needed for accuracy, especially when only low-mode response is of interest. For these reasons unconditionally stable algorithms are generally preferred.

A fundamental result, due to Dahlquist [6] (see also Krieg [16]), is that there is no unconditionally stable explicit method amongst the class of linear multistep methods. Thus attribute 1 necessitates the use of implicit methods, and this engenders considerable computational effort since coefficient matrices must be stored and factored. It is important for purposes of efficiency that this work be kept to a minimum. This can be done by insisting that the solution of no more than one implicit system, of the size of the mass and stiffness matrices, be required at each time step. More elaborate schemes have been proposed which require larger implicit systems, or two, or more, implicit systems of the size of the stiffness and mass to be solved at each step, and improved properties have been obtained (see for example Argyris, Dunne and Angelopoulos [1], Geradin [8], Hilber [11], Krieg and Key [17], and Kurdi [18]). However, these techniques require at least twice the storage and computational effort of the simpler methods and thus have not been widely adopted.

Experience has indicated that in structural dynamics second-order accurate methods are vastly superior to first-order accurate methods. Another result due to Dahlquist [6] is that there is no third-order accurate unconditionally stable linear multistep method. Thus we must be content with second-order accuracy. Furthermore, the second-order method with the smallest error constant is the trapezoidal rule.* Hence any effort to obtain some specific property within the context of second-order accurate unconditionally stable methods must result in some degradation of accuracy when compared with trapezoidal rule. It is important to be aware of this since numerical dissipation is another desirable characteristic and one not possessed by trapezoidal rule. (Numerical dissipation is used to damp out any spurious participation of the higher modes.)

Some writers continue to suggest that a viscous damping term be added to suppress higher modes, but it is well known that the interaction between the viscous term and typical implicit integrators results in virtually no dissipation in the higher modes (see [3,11,15]).

It is also desirable that an algorithm be self-starting, since our understanding of ones that are not is generally obscured. For example, if an algorithm requires a distinct starting procedure we must analyze the starting procedure in addition to the algorithm, and also the interaction of the algorithm with all possible values generated by the starting procedure. A distinct starting procedure may also engender additional coding and computational effort.

Algorithms which are not self-starting involve data from more than two time steps to advance the solution. This requires additional storage, and since no matter how many steps we include we are restricted to at most second-order accuracy, a point of diminishing return is quickly reached. Furthermore, it is possible to achieve all the aforementioned attributes within a one-step method (i.e., a method for which the displacements, velocities and accelerations at one step, along with the given forces, suffice to advance the solution to the next step). Thus it seems that the second-order accurate, unconditionally stable, one-step method which achieves the optimal balance between effective numerical dissipation and loss of accuracy compared with trapezoidal rule, is the desired algorithm for most problems of structural dynamics.

The Newmark family of algorithms [19] enjoys wide use in structural engineering, but attributes 3 and 4 cannot exist simultaneously within this family. (Second-order accuracy requires $\gamma = 1/2$ which precludes dissipation.)

In 1968 Wilson [22] developed the first method which essentially satisfied attributes 1-5. As the algorithm possessed excessive low-

mode dissipation (i.e., loss of accuracy) several efforts were made by Wilson and co-workers to improve it [3,7]. In these efforts it was seen how to control, to some extent, the amount of dissipation. However, it was not possible within the scheme to continuously reduce to zero dissipation, and the least damped member of the family still possessed more low-mode dissipation than desired. The key idea employed in the development of the so-called Wilson θ method was the satisfaction of the equations of motion outside the time interval in question at the θ , or collocation, point.

Subsequently a very peculiar property of the Wilson method was discovered numerically by Goudreau and Taylor [10], i.e., a tendency to significantly overshoot exact solutions to initial value problems in the early response when large time steps are employed. Since such tests reflect how the higher modes will behave in multidegree-of-freedom problems involving impact or suddenly applied loads, the Wilson method has since been considered inappropriate for such applications. Additional attention has been drawn to this feature by Argyris, Dunne and Angelopoulos [2] and Ghose [9].

We have undertaken a research study to ascertain if improved collocation schemes can be developed along the lines enumerated in attributes 1-5 and not subject to the above pitfall. In Section 2 we describe the considered family of methods which represents a systematic generalization of the Wilson collocation idea and contains the θ methods as special cases. In Sections 2.1-2.3 we determine the accuracy, stability, dissipation and dispersion characteristics of the new methods. The results of the analyses indicate an optimal one-parameter family of collocation schemes. In particular, we are able to find an optimal value of θ for Wilson's method which results in improved properties over the value $\theta = 1.4$ advocated in [3].

In Section 3 we review a one-parameter family of algorithms, α methods, recently proposed in [12] which also satisfies attributes 1-5. Parameter value $\alpha = 0$ corresponds to the trapezoidal rule and decreasing α increases the amount of numerical dissipation. The concept employed in developing these algorithms was to combine two different forms of numerical dissipation in such a way that second-order accuracy and improved damping are obtained. The resultant algorithm represents only a minor modification of the Newmark family. It was found in [12] that the α methods represented an improvement over the Wilson θ methods.

In Section 4 we compare the optimal collocation and α methods. Also included in the comparison are the Houbolt [13] and Park [20] methods. It is found that, on the basis of the standard measures (e.g. algorithmic damping ratio, relative period error, etc.) α methods are superior.

In Section 5 we present a discussion of overshoot. It is argued that a tendency to overshoot will not be detected by the traditionally employed measures of stability and accuracy, and thus must

* The trapezoidal rule also goes under the aliases (constant) average acceleration method, Crank-Nicolson method, and Chan-Cox-Benfield method.

be considered separately. In Section 5.1 the basis for studying overshooting is developed. In Section 5.2 the optimal collocation schemes and α methods are compared with respect to overshoot. It is found that pathological overshooting is an inherent property of collocation. On the other hand, the α methods are shown to exhibit good overshooting characteristics.

The present developments are summarized in Section 6.

2. Collocation Schemes

The linear undamped matrix equation of structural dynamics is

$$\underline{M}\ddot{\underline{u}} + \underline{K}\underline{u} = \underline{F} \quad (2.1)$$

where \underline{M} is the mass matrix, \underline{K} is the stiffness matrix, \underline{F} is the vector of applied loads (a given function of time), \underline{u} is the displacement vector and superposed dots indicate time differentiation (e.g. $\ddot{\underline{u}} = d^2\underline{u}/dt^2$ is the acceleration vector). The initial-value problem consists of finding a function $\underline{u} = \underline{u}(t)$ satisfying (2.1) for all $t \in [0, \tau]$, $\tau > 0$, and the initial conditions

$$\underline{u}(0) = \underline{d} \quad (2.2)$$

$$\dot{\underline{u}}(0) = \underline{v} \quad (2.3)$$

where \underline{d} and \underline{v} are given vectors of initial data.

Consider the following family of one-step difference methods for obtaining approximate solutions of the initial-value problem:

$$\underline{M}\underline{a}_{n+\theta} + \underline{K}\underline{d}_{n+\theta} = \underline{F}_{n+\theta} \quad (2.4)$$

$$\underline{a}_{n+\theta} = (1 - \theta)\underline{a}_n + \theta\underline{a}_{n+1} \quad (2.5)$$

$$\underline{d}_{n+\theta} = \underline{d}_n + \theta\Delta t \underline{v}_n + (\theta\Delta t)^2 [(1/2 - \beta)\underline{a}_n + \beta\underline{a}_{n+\theta}] \quad (2.6)$$

$$\underline{F}_{n+\theta} = (1 - \theta)\underline{F}_n + \theta\underline{F}_{n+1} \quad (2.7)$$

$$\underline{d}_{n+1} = \underline{d}_n + \Delta t \underline{v}_n + \Delta t^2 [(1/2 - \beta)\underline{a}_n + \beta\underline{a}_{n+1}] \quad (2.8)$$

$$\underline{v}_{n+1} = \underline{v}_n + \Delta t [(1 - \gamma)\underline{a}_n + \gamma\underline{a}_{n+1}] \quad (2.9)$$

$$\underline{d}_0 = \underline{d} \quad (2.10)$$

$$\underline{v}_0 = \underline{v} \quad (2.11)$$

$$\underline{a}_0 = \underline{M}^{-1}(\underline{F}_0 - \underline{K}\underline{d}_0) \quad (2.12)$$

where $n \in \{0, 1, \dots, N-1\}$, N is the number of time steps, $\Delta t = \tau/N$, \underline{d}_n , \underline{v}_n and \underline{a}_n are the approximations to $\underline{u}(t_n)$, $\dot{\underline{u}}(t_n)$ and $\ddot{\underline{u}}(t_n)$, respectively, in which $t_n = n\Delta t$, $\underline{F}_n = \underline{F}(t_n)$, and β , γ and θ are free parameters which govern the accuracy and stability of the algorithms. If $\theta = 1$ this family reduces to the Newmark family. If $\beta = 1/6$ and $\gamma = 1/2$ the Wilson θ methods are obtained. We call the above methods collocation schemes and θ the collocation parameter.

Characteristics of the preceding algorithms can be ascertained by considering the homogeneous

single-degree-of-freedom model equation

$$\underline{M}\ddot{\underline{x}} + \underline{K}\underline{x} = 0 \quad (2.13)$$

In this case (2.4) - (2.9) can be succinctly written

$$\underline{x}_{n+1} = \underline{A}\underline{x}_n \quad (2.14)$$

where

$$\underline{x}_n = (d_n, \Delta t v_n, \Delta t^2 a_n)^T \quad (2.15)$$

and \underline{A} is called the amplification matrix. Many important properties of an algorithm may be determined from the spectral properties of its amplification matrix. The characteristic equation for \underline{A} is

$$-\det(\underline{A} - \lambda \underline{I}) = \lambda^3 - 2A_1\lambda^2 + A_2\lambda - A_3 = 0 \quad (2.16)$$

where \underline{I} is the identity matrix, λ denotes an eigenvalue of \underline{A} and

$$A_1 = \frac{1}{2} \text{trace } \underline{A} \quad (2.17)$$

$$A_2 = \text{sum of principal minors of } \underline{A} \quad (2.18)$$

$$A_3 = \text{determinant } \underline{A} \quad (2.19)$$

are invariants of \underline{A} .

The spectral radius $\rho = \max\{|\lambda_1|, |\lambda_2|, |\lambda_3|\}$, where λ_1 , λ_2 and λ_3 are the eigenvalues of \underline{A} .

The explicit definition of \underline{A} for the family of algorithms defined by (2.4) - (2.9) is

$$\underline{A} = \begin{bmatrix} 1 + \beta A_{31} & 1 + \beta A_{32} & \frac{1}{2} + \beta(A_{33} - 1) \\ \gamma A_{31} & 1 + \gamma A_{32} & 1 + \gamma(A_{33} - 1) \\ A_{31} & A_{32} & A_{33} \end{bmatrix} \quad (2.20)$$

where

$$A_{31} = -\Omega^2/D \quad (2.21)$$

$$A_{32} = -\theta\Omega^2/D \quad (2.22)$$

$$A_{33} = 1 - (1 + \theta^2\Omega^2/2)/D \quad (2.23)$$

$$D = \theta(1 + \beta\theta^2\Omega^2) \quad (2.24)$$

$$\Omega = \omega\Delta t \quad (2.25)$$

$$\omega = (K/M)^{1/2} \quad (2.26)$$

The corresponding invariants are

$$A_1 = 1 - \Omega^2(\gamma + \theta - 1/2)/(2D) + A_3/2 \quad (2.27)$$

$$A_2 = 1 - \Omega^2(\gamma + \theta - 3/2)/D + 2A_3 \quad (2.28)$$

$$A_3 = (\theta - 1)[1 + \Omega^2(\beta(\theta^2 + \theta + 1) - \gamma - (\theta - 1)/2)]/D \quad (2.29)$$

The velocities and accelerations may be eliminated by repeated use of (2.14) to obtain a difference equation in terms of displacements:

$$d_{n+1} - 2A_1 d_n + A_2 d_{n-1} - A_3 d_{n-2} = 0, \quad n \in \{2, 3, \dots, N-1\}. \quad (2.30)$$

Comparison of (2.30) with (2.16) indicates that the discrete solution has the representation

$$d_n = \sum_{i=1}^3 c_i \lambda_i^n \quad (2.31)$$

where coefficients c_1 , c_2 and c_3 are determined by the initial data. It is to be noted that (2.31) is the general solution of (2.30) only if the eigenvalues are distinct. If this is not the case a slightly different representation is appropriate. For example, if $\lambda_1 = \lambda_2$, then the general solution of (2.30) is

$$d_n = (c_1 + nc_2)\lambda_1^n + c_3\lambda_3^n \quad (2.32)$$

whereas if $\lambda_1 = \lambda_2 = \lambda_3$ then the general solution is

$$d_n = (c_1 + nc_2 + n^2 c_3)\lambda_1^n. \quad (2.33)$$

2.1. Consistency and Accuracy

The local truncation error of (2.30) is

$$\sigma = [u(t + \Delta t) - 2A_1 u(t) + A_2 u(t - \Delta t) - A_3 u(t - 2\Delta t)]/\Delta t^2 \quad (2.34)$$

where u satisfies (2.13). Expanding u about t in (2.34) yields

$$\sigma = \sum_{i=0}^m T_i \Delta t^{i-2} u^{(i)}(t) + O(\Delta t^{m-1}) \quad (2.35)$$

where $u^{(i)}$ denotes the i^{th} derivative of u and

$$T_0 = 1 - 2A_1 + A_2 - A_3 \quad (2.36)$$

$$T_i = [1 + (-1)^i A_2 - (-2)^i A_3]/i!, \quad i > 0. \quad (2.37)$$

The difference equation (2.30) is said to be consistent with the differential equation (2.13) if $\sigma = O(\Delta t^k)$ in which $k > 0$; k is called the order of accuracy.

Since u satisfies (2.13) all derivatives in (2.35) of second and higher order can be eliminated. For example, setting $m = 4$ in (2.35) and employing (2.13) yields

$$\sigma = [\Omega^{-2} T_0 - T_2 + \Omega^2 T_4] \omega^2 u + [\Omega^{-1} T_1 - \Omega T_3] \omega \dot{u} + O(\Delta t^3). \quad (2.38)$$

In (2.38), T_0 to T_4 may be explicated by way of (2.27) - (2.29), (2.36) and (2.37), viz.

$$T_0 = \Omega^2/D \quad (2.39)$$

$$T_1 = \Omega^2(\theta + \gamma - 3/2)/D \quad (2.40)$$

$$T_2 = 1 - T_1/2 - A_3 \quad (2.41)$$

$$T_3 = T_1/6 + A_3 \quad (2.42)$$

$$T_4 = 1/12 - T_1/24 - 7A_3/12. \quad (2.43)$$

Employing the above in (2.38) reveals that

$$\sigma = \Omega \omega \dot{u} (\gamma - 1/2)/D + O(\Delta t^2). \quad (2.44)$$

Thus with no restrictions on β , γ and θ , the difference equation is consistent and first-order accurate. However, if $\gamma = 1/2$ the order of accuracy is at least 2. Assuming this is the case, (2.38) becomes

$$\sigma = \Omega^2 \omega^2 u [1 - 12\beta - 6\theta(\theta - 1)]/(12D) + O(\Delta t^3) \quad (2.45)$$

from which it follows that if, in addition,

$$\beta = 1/12 - \theta(\theta - 1)/2 \quad (2.46)$$

then the order of accuracy is at least 3.

We are only interested in methods which are at least second-order accurate. Thus in the subsequent discussion it is assumed $\gamma = 1/2$.

2.2. Stability

A matrix \underline{A} is stable if $\rho \leq 1$ and eigenvalues λ of multiplicity greater than one satisfy $|\lambda| < 1$.

The condition of stability that we shall require of the family of algorithms (2.4) - (2.9) is that the associated amplification matrix \underline{A} be stable.

If \underline{A} is stable for all $\Omega \in [0, \Omega_c]$, where Ω_c is a positive constant, stability is said to be conditional, whereas if \underline{A} is stable for all $\Omega \in [0, \infty)$, stability is said to be unconditional. In the sequel we shall only be concerned with determining the values of the parameters β and θ for which unconditional stability holds. (Keep in mind that it is assumed $\gamma = 1/2$.)

Remarks. 1. The requirement that eigenvalues λ of multiplicity greater than one satisfy $|\lambda| < 1$ can be seen to be necessary by comparing (2.31) - (2.33). Otherwise linear or quadratic growth in n is possible (so-called weak instabilities).

2. By Lax's equivalence theorem [21], a consistent, conditionally stable algorithm as above is convergent (i.e., for t_n fixed and $n = t_n/\Delta t$, $d_n \rightarrow u(t_n)$ as $\Delta t \rightarrow 0$).

Conditions under which eigenvalues of magnitude one occur can be examined by substituting $\lambda = e^{i\alpha}$ into (2.16) where $\alpha \in [0, 2\pi)$. Since the real and imaginary parts of the resulting equation must be zero individually we get

$$\cos \alpha (1 - 4 \sin^2 \alpha - 4A_1 \cos \alpha + A_2) + 2A_1 - A_3 = 0 \quad (2.47)$$

$$\sin \alpha (1 - 4 \cos^2 \alpha + 4A_1 \cos \alpha - A_2) = 0 \quad (2.48)$$

There are three cases:

- (i) $\alpha = 0$. This corresponds to $\lambda = 1$ and results in

$$1 - 2A_1 + A_2 - A_3 = 0 \quad (2.49)$$

- (ii) $\alpha = \pi$. This corresponds to $\lambda = -1$ and yields

$$1 + 2A_1 + A_2 + A_3 = 0 \quad (2.50)$$

- (iii) All remaining values of α correspond to complex eigenvalues. Manipulating (2.47) and (2.48) to eliminate α results in

$$1 - A_2 + 2A_1A_3 - A_3^2 = 0 \quad (2.51)$$

Substitution of (2.27) - (2.29) into (2.49) reveals that $\lambda = 1$ if and only if $\Omega = 0$. In this limiting case the eigenvalues of A are $\lambda_1 = \lambda_2 = 1$ and $\lambda_3 = 1 - 1/\theta$.

Proceeding in a similar fashion with (2.50), we conclude that if $\theta \geq 1$ and $\beta \geq (2\theta^2 - 1)/(4(2\theta^3 - 1))$, then no $\Omega \in [0, \infty)$ exists such that $\lambda = -1$. However, if $\beta = (2\theta^2 - 1)/(4(2\theta^3 - 1))$, then $\lambda \rightarrow -1$ as $\Omega \rightarrow \infty$.

Finally, from (2.51) we determine that if $\theta > 1$ and $\beta < \theta/(2(\theta + 1))$, then there exists no solution $\Omega \in [0, \infty)$ such that $|\lambda| \geq 1$. On the other hand, if $\theta \geq 1$ and $\beta = \theta/(2(\theta + 1))$, then (2.51) is trivially satisfied for all Ω . In this case A has complex conjugate eigenvalues of magnitude 1 and the real eigenvalue $1 - 1/\theta$.

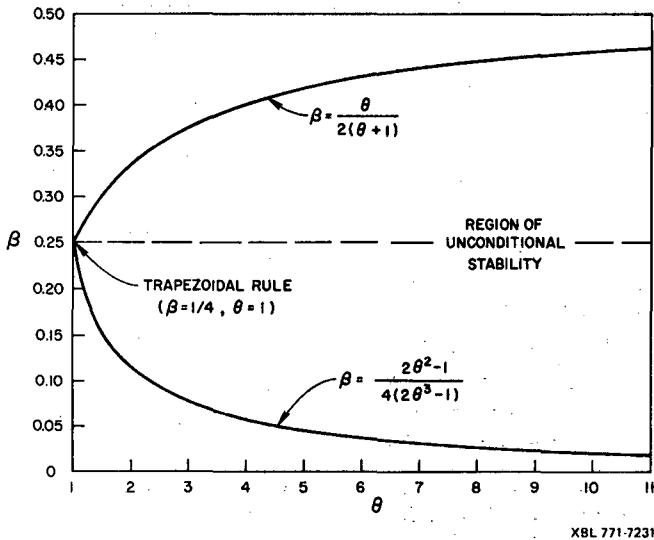


Figure 1. Region of unconditional stability for collocation schemes.

In summary, the conditions for unconditional stability are (see Figure 1):

$$\theta \geq 1, \quad \frac{\theta}{2(\theta + 1)} \geq \beta \geq \frac{2\theta^2 - 1}{4(2\theta^3 - 1)} \quad (2.52)$$

By comparing (2.46) and (2.52) we see that the schemes which are third-order accurate cannot be unconditionally stable.

2.3. Numerical Dissipation and Dispersion

A consequence of convergence is the existence of a positive constant $\bar{\Omega}$ such that if $\Omega \in (0, \bar{\Omega})$, then there are two complex conjugate eigenvalues of A , $\lambda_{1,2}$, called principal roots, and a so-called spurious root λ_3 , which satisfy $|\lambda_3| < |\lambda_{1,2}| \leq 1$. When this is the case, the solution of (2.30) may be written in the form

$$d_n = e^{-\bar{\xi}\bar{\omega}t} (c_1 \cos \bar{\omega}t_n + c_2 \sin \bar{\omega}t_n) + c_3 \lambda_3^n \quad (2.53)$$

where

$$\lambda_{1,2} = A \pm Bi = e^{\bar{\Omega}(-\bar{\xi} \pm i)} \quad (2.54)$$

$$\bar{\omega} = \bar{\Omega}/\Delta t \quad (2.55)$$

$$\bar{\xi} = -\ln(A^2 + B^2)/(2\bar{\Omega}) \quad (2.56)$$

$$\bar{\Omega} = \arctan(B/A) \quad (2.57)$$

The measures of numerical dissipation and dispersion that we employ are the algorithmic damping ratio $\bar{\xi}$ (see [12]) and relative period error $(\bar{T} - T)/T$, respectively, where $T = 2\pi/\omega$ and $\bar{T} = 2\pi/\bar{\omega}$. Both these quantities are defined in terms of the principal roots and thus are meaningful only for $\Omega < \bar{\Omega}$. Outside this region accuracy is not an issue and we are concerned only about stability and dissipation. Here ρ is an important measure since it provides information about stability and dissipation.

Figure 2 illustrates the behavior of spectral radii versus $\Delta t/T$ for some unconditionally stable

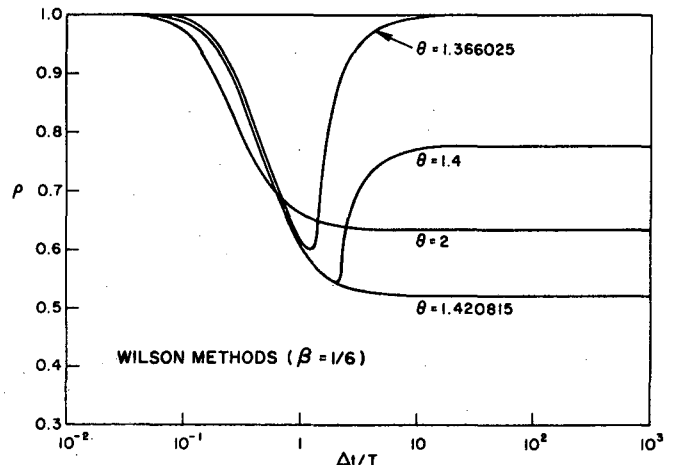


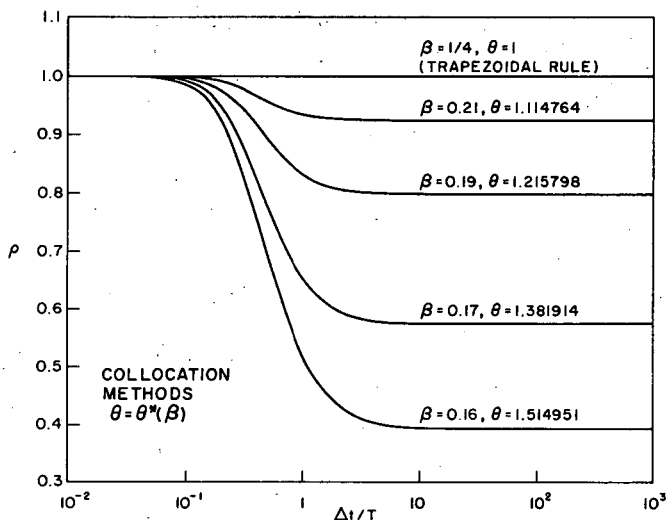
Figure 2. Spectral radii for Wilson θ methods.

members of the Wilson θ method. The value $\theta = 1.366025$ is the smallest θ within the region of unconditional stability (cf. (2.52)). For this value $\rho \rightarrow 1$ as $\Delta t/T \rightarrow \infty$. This behavior, predicted by the stability analysis, is typical of all schemes for which (θ, β) lie upon the lower stability curve of Figure 1, and is highly undesirable since there is no numerical dissipation in the higher modes. Increasing the value of θ for fixed β decreases the limit of ρ as $\Delta t/T \rightarrow \infty$ (e.g. the $\theta = 1.4$ curve in Figure 2). The point along the curve at which ρ achieves its minimum marks the bifurcation of the complex conjugate principal roots into real roots. The smallest value of θ for which the principal roots remain complex at all $\Delta t/T$ is found to be $\theta = 1.420815$. Note the vastly superior spectral properties of $\theta = 1.420815$ over $\theta = 1.4$ (cf. [3]). As θ is further increased the limiting value of ρ decreases until it achieves a minimum and then begins to increase again (see for example $\theta = 2$ in Figure 2). The behavior of ρ in Figure 2 is typical for all $\beta \in (0, 1/4)$.

As β decreases, θ must increase rapidly to maintain unconditional stability. So as not to incur too large a value of θ we shall restrict our attention to the regime $\beta > .16$. We shall also present arguments later on which indicate that β may as well be assumed to be less than or equal to $1/4$.

Let $\theta^* = \theta^*(\beta)$ denote the smallest value of θ for which the principal roots remain complex as $\Delta t/T \rightarrow \infty$. Values of θ^* , obtained numerically for various values of β , are presented in Table 1, along with the corresponding algorithmic damping ratios and relative period errors for $\Delta t/T = .1$. The points (θ^*, β) lie slightly above the lower stability boundary of Figure 1. Note that both the damping ratio and period error increase as β decreases.

In Figure 3 spectral radii of some of the tabulated cases are illustrated. Note that in each

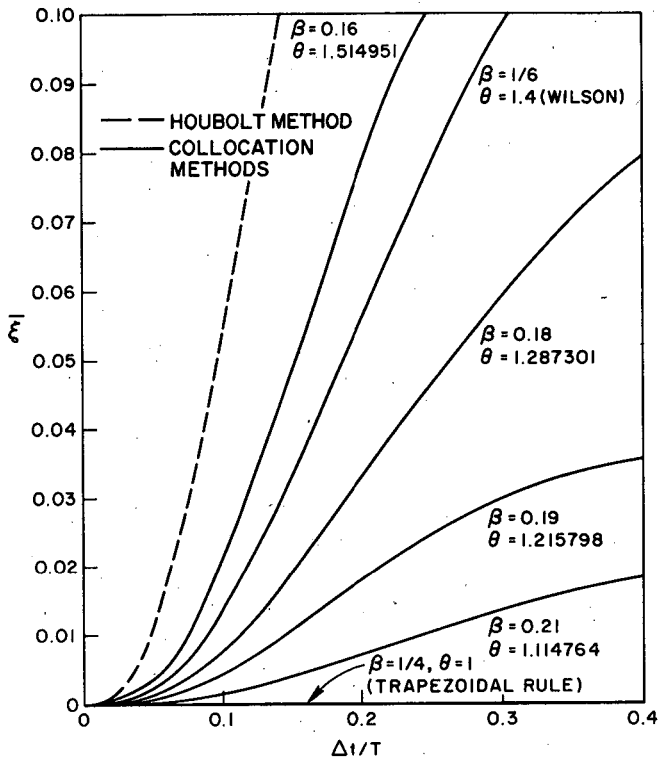


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Figure 3. Spectral radii for optimal collocation schemes.

case the minimum value of ρ is obtained as $\Delta t/T \rightarrow \infty$, a desirable feature in multidegree-of-freedom applications.

In Figure 4 algorithmic damping ratios are plotted. The continuous control of numerical dissipation in the considered family of algorithms is evident. The damping ratios of the Wilson and Houbolt methods are also depicted in Figure 4 for comparison purposes.



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Figure 4. Algorithmic damping ratios for collocation schemes and Houbolt method.

The relative period errors for the various cases are presented in Figure 5. Clearly, for a fixed value of $\Delta t/T$ the relative period errors increase with θ .

An investigation revealed that for β and $\Delta t/T$ fixed, such that $\Omega < \bar{\Omega}$, as θ is increased beyond θ^* both the damping ratio and period error increase quadratically with θ . On the other hand, for θ fixed and β increasing from the lower unconditional stability limit to the upper one (see (2.52) and Figure 1), the damping ratio decreases in a linear fashion from its maximum value to zero, whereas the period error increases linearly. Again this holds for all $\Omega < \bar{\Omega}$. Thus we conclude: The best unconditionally stable algorithms, providing a maximum of dissipation and minimum period error are obtained if $\theta = \theta^*(\beta)$. We call such methods optimal collocation methods and restrict subsequent attention to these schemes. Some pairs $(\beta, \theta^*(\beta))$ are listed in Table 1 and intermediate points can be determined by linear interpolation.

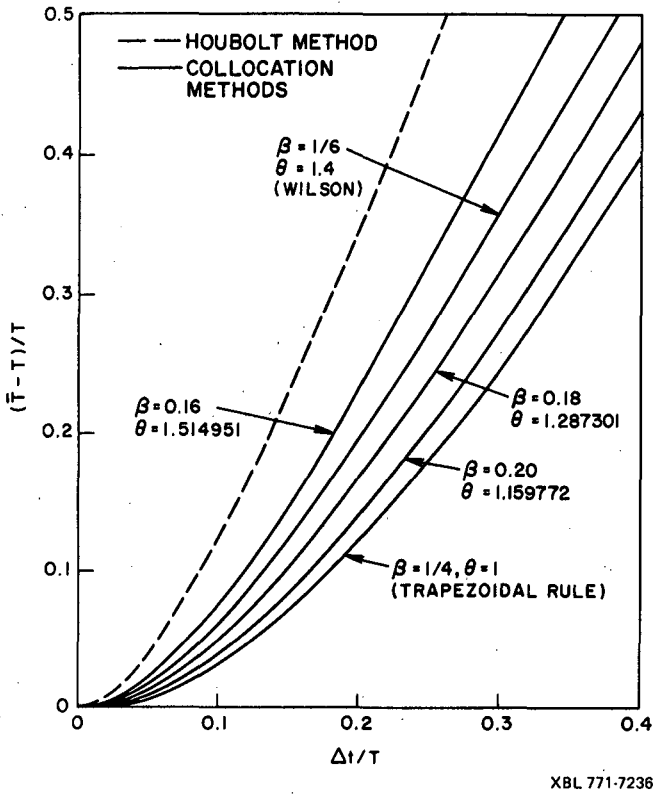


Figure 5. Relative period errors for collocation schemes and Houbolt method.

Table 1. Smallest collocation parameter which insures complex conjugate principal roots as $\Delta t/T \rightarrow \infty$. Corresponding values of algorithmic damping ratio and relative period error for $\Delta t/T = .1$.

β	θ^*	ξ	$(\bar{T}-T)/T$
1/4	1	0	.032
.24	1.021712	.60 x 10 ⁻⁴	.032
.23	1.047364	.27 x 10 ⁻³	.033
.22	1.077933	.70 x 10 ⁻³	.034
.21	1.114764	.14 x 10 ⁻²	.036
.20	1.159772	.27 x 10 ⁻²	.039
.19	1.215798	.46 x 10 ⁻²	.043
.18	1.287301	.77 x 10 ⁻²	.050
.17	1.381914	.13 x 10 ⁻¹	.060
1/6	1.420815	.15 x 10 ⁻¹	.064
.16	1.514951	.21 x 10 ⁻¹	.075

3. α Method

To improve upon the numerical dissipation properties of the Newmark family of algorithms, we introduced in [12] a one-parameter family of algorithms given as follows:

$$M \ddot{a}_{n+1} + (1 + \alpha)K \ddot{d}_{n+1} - \alpha K \ddot{d}_n = F_{n+1} \quad (3.1)$$

$$\ddot{d}_{n+1} = \ddot{d}_n + \Delta t \ddot{v}_n + \Delta t^2 [(1/2 - \beta) \ddot{a}_n + \beta \ddot{a}_{n+1}] \quad (3.2)$$

$$\ddot{v}_{n+1} = \ddot{v}_n + \Delta t [(1 - \gamma) \ddot{a}_n + \gamma \ddot{a}_{n+1}] \quad (3.3)$$

$$\ddot{d}_0 = \ddot{d} \quad (3.4)$$

$$\ddot{v}_0 = \ddot{v} \quad (3.5)$$

$$\ddot{a}_0 = M^{-1}(F_0 - K \ddot{d}_0) \quad (3.6)$$

where $n \in \{0, 1, \dots, N - 1\}$, $\gamma = (1 - 2\alpha)/2$, $\beta = (1 - \alpha)^2/4$ and $\alpha \in [-1/3, 0]$. For $\alpha = 0$ we have the well known trapezoidal rule which is undamped. Decreasing α increases the amount of numerical dissipation. For each value of α in the admissible range, the algorithm in question is unconditionally stable and second-order accurate. For details of the stability and accuracy analysis see [11] and [12].

4. Comparison of Dissipative Schemes

In this section we compare algorithms which have the following features in common:

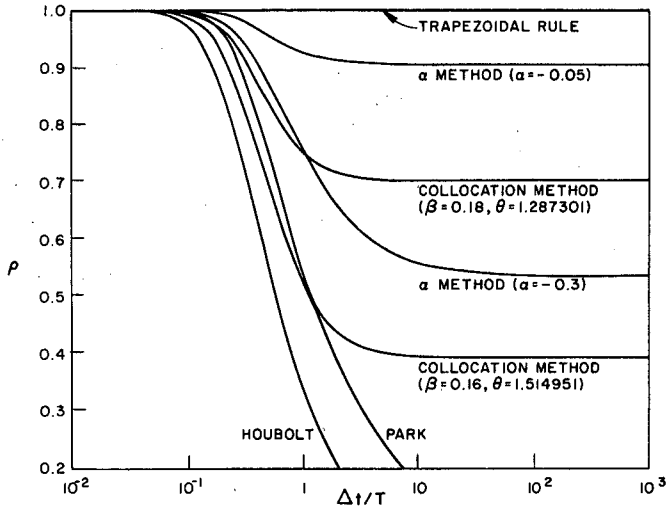
- (i) They are implicit in m unknowns, where m is the dimension of y . Thus the methods considered require roughly the same computational effort per time step.
- (ii) They are unconditionally stable.
- (iii) They are second-order accurate.

Requirement (i) excludes, for example, the unconditionally stable scheme presented in [1], since it requires the solution of an implicit system of dimension $2m$. Explicit schemes are precluded by (ii) and dissipative Newmark schemes ($\gamma > 1/2$) are eliminated by requirement (iii).

The algorithms considered are:

- a. Houbolt's method [13].
- b. Park's method [20].
- c. Optimal collocation schemes of Section 2.
- d. α methods of Section 3.

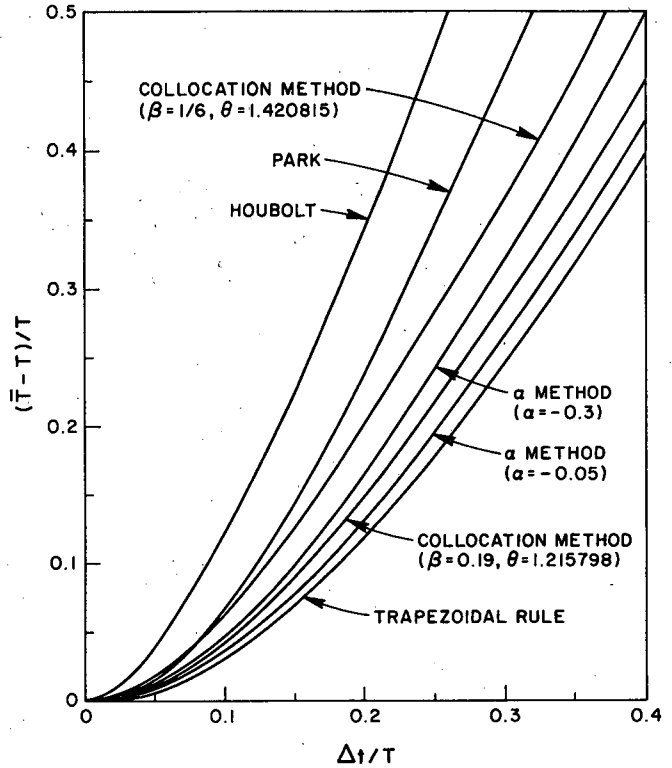
The Houbolt and Park methods do not permit parametric control of the amount of dissipation present, whereas the collocation schemes and α methods do. In addition, the Houbolt and Park methods require starting procedures since they are multistep methods, whereas the collocation schemes and α methods are self-starting.



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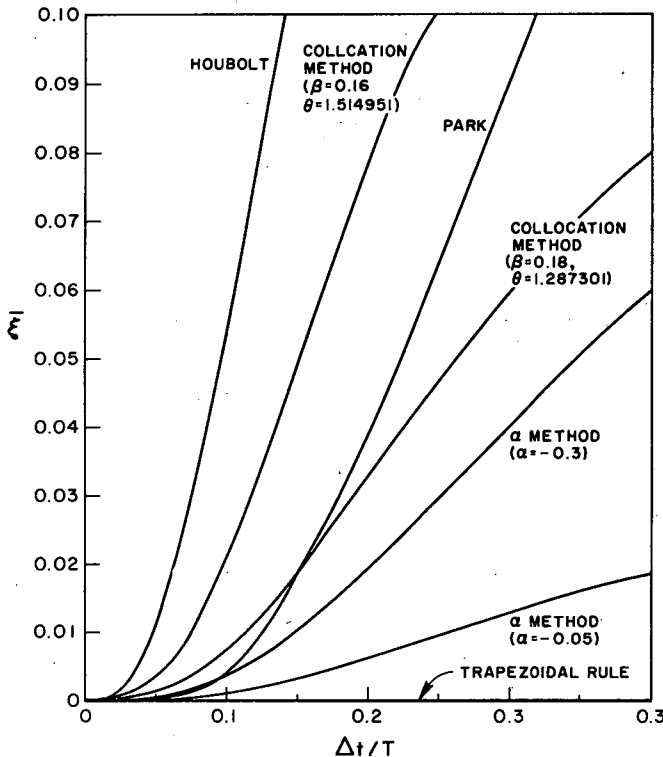
Figure 6. Spectral radii for α methods, optimal collocation schemes and Houbolt and Park methods.

In Figure 6 the spectral radii of the various cases are presented. The spectral radii of the Houbolt and Park methods approach zero as $\Delta t/T \rightarrow \infty$. This is typical of backward difference schemes. Collocation schemes and α methods are seen also to possess strong damping in the high frequency regime. Recall that the effect of $\rho < 1$ is accumulative, e.g. $\rho^n < e^{-n(1-\rho)}$, which rapidly approaches zero as n is increased.



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Figure 8. Relative period errors for α methods, optimal collocation schemes, and Houbolt and Park methods.



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Figure 7. Algorithmic damping ratios for α methods, optimal collocation schemes, and Houbolt and Park methods.

In Figure 7 algorithmic damping ratios are compared. The Houbolt and collocation methods are seen to affect the low modes (i.e., $\Delta t/T \leq .1$) too strongly. The inefficiency of the damping in the collocation scheme versus the α scheme can be seen by comparing the cases $\beta = .18$ and $\alpha = -.3$, respectively. From Figure 6, $\alpha = -.3$ is seen to damp the high modes more strongly than $\beta = .18$. On the other hand, from Figure 7 the low modes are affected less by $\alpha = -.3$ than by $\beta = .18$.

Relative period errors are compared in Figure 8. The collocation schemes and α methods have smaller errors than the Houbolt and Park methods.

The following observations summarize the comparisons:

All methods are capable of sufficiently damping out the high modes. The Houbolt method affects the low modes much too strongly, both from the point of view of damping ratio and of period error. Park's method possesses good low mode damping properties, however its period error is higher than the collocation schemes and α methods. The collocation schemes damp the low-modes too strongly. The α methods, on balance, emerge as the best amongst the methods considered.

5. Overshoot

In [10] Goudreau and Taylor discovered a peculiar property of the Wilson θ method. Despite the method's unconditional stability, numerical experiments revealed a tendency to significantly 'overshoot' exact solutions in the first few steps. More recently Argyris, et al. [2] and Ghose [9] have drawn attention to this behavior.

In this section we present an analysis of this phenomenon and then compare the considered schemes on this basis.

5.1. General Concepts

We begin with a discussion of the concept of stability. Recall that stability is defined with respect to the spectral properties of the amplification matrix \tilde{A} (see Section 2.2). Typically, the eigenvalues are distinct and in this case \tilde{A} admits the decomposition

$$\tilde{A} = \tilde{P} \tilde{\Lambda} \tilde{P}^{-1} \quad (5.1)$$

where \tilde{P} is a matrix of eigenvectors and $\tilde{\Lambda}$ is a diagonal matrix of eigenvalues. With the aid of (5.1) the solution of (2.14) may be expressed as

$$\tilde{x}_n = \tilde{A}^n \tilde{x}_0 = \tilde{P} \tilde{\Lambda}^n \tilde{P}^{-1} \tilde{x}_0. \quad (5.2)$$

Let $\|\cdot\|$ denote any norm such that $\|\tilde{\Lambda}\| = \rho$. As we may scale \tilde{P} in any way we like, let $\|\tilde{P}\| = 1$. Multiplying (5.2) by \tilde{P}^{-1} and taking the norm of both sides results in

$$\|\tilde{P}^{-1} \tilde{x}_n\| \leq \rho^n \|\tilde{P}^{-1} \tilde{x}_0\|. \quad (5.3)$$

Thus if $\rho = 1$, $\|\tilde{P}^{-1} \tilde{x}_n\|$ is uniformly bounded by its initial value; if $\rho < 1$, $\|\tilde{P}^{-1} \tilde{x}_n\| \rightarrow 0$ as $n \rightarrow \infty$. From these results one might be inclined to think that no growth of \tilde{x}_n is possible. However, taking the norm of both sides of (5.2) yields

$$\|\tilde{x}_n\| \leq \rho^n \|\tilde{P}^{-1}\| \|\tilde{x}_0\|, \quad (5.4)$$

which reveals that $\|\tilde{P}^{-1}\|$ must be considered when comparing $\|\tilde{x}_n\|$ with $\|\tilde{x}_0\|$. Here, if $\rho = 1$, $\|\tilde{x}_n\|$ is uniformly bounded by $\|\tilde{P}^{-1}\| \|\tilde{x}_0\|$, but if $\rho < 1$, then $\|\tilde{x}_n\| \rightarrow 0$ as $n \rightarrow \infty$. The latter case corresponds to the dissipative algorithms under consideration in this paper and thus we see that the spectral properties of \tilde{A} determine the asymptotic behavior of $\|\tilde{x}_n\|$ as $n \rightarrow \infty$. On the other hand, it is the size of $\|\tilde{P}^{-1}\|$ which must concern us for small n .

For a stable amplification matrix

$$\|\tilde{A}^n\| \leq \|\tilde{P}^{-1}\| \quad (5.5)$$

and thus we have the sharper bound

$$\|\tilde{x}_n\| \leq \|\tilde{A}^n\| \|\tilde{x}_0\|. \quad (5.6)$$

From (5.4) we deduce that the crudest bound occurs if $n = 1$, which along with (5.6) suggests that it is $\|\tilde{A}\|$ which governs the potential for early growth, i.e., 'overshoot.'

A simple example indicates that the norm of a matrix may be arbitrarily large even though the spectral radius is very small. Let

$$\tilde{A} = \begin{bmatrix} \epsilon & k \\ 0 & \epsilon \end{bmatrix} \quad (5.7)$$

where $0 < \epsilon < 1$ and $k \gg 1$. The spectral radius of \tilde{A} is ϵ whereas $\|\tilde{A}\| \approx k$. The effect of the spectral radius as $n \rightarrow \infty$ is evident from

$$\tilde{A}^n = \begin{bmatrix} \epsilon^n & n\epsilon^{n-1}k \\ 0 & \epsilon^n \end{bmatrix} \quad (5.8)$$

in which all terms go to zero as $n \rightarrow \infty$. However, due to the presence of k , the term $n\epsilon^{n-1}k$, is very large for n small enough.

From this example and the previous discussion we draw the following conclusions:

1. The long term, or asymptotic, behavior of \tilde{x}_n is governed by the spectral properties of \tilde{A} .
2. The short term behavior of \tilde{x}_n is governed by the norm of \tilde{A} .
3. A stable matrix \tilde{A} may have arbitrarily large norm.

Thus, in addition to the measures of stability and accuracy considered in Section 2, it is important to examine the norm of an amplification matrix to see if there is a tendency to overshoot. Since the norm of a matrix depends upon every entry, a term-by-term evaluation may be employed. Specifically, pick d and v , compute d_1 and v_1 over the full range of Ω for the given method, and compare d_1 and v_1 with u_{\max} and \dot{u}_{\max} , respectively, where the latter are the maximum absolute values of the exact solutions for the given initial conditions.

Another possibility is to work in terms of the natural energy norm of the problem at hand, viz.,

$$E_n = \|(d_n, v_n)\|_E^2 = (Mv_n^2 + Kd_n^2) / 2. \quad (5.9)$$

For exact solutions of (2.13),

$$\|(u(t), \dot{u}(t))\|_E = \|(d, v)\|_E. \quad (5.10)$$

for all t . Comparison of $\|(d_1, v_1)\|_E$ with $\|(d, v)\|_E$ for varying Ω will also reveal any overshoot.

Before assessing the collocation schemes and α methods on the basis of the preceding ideas, we note that the overshoot analysis of multistep methods, such as Houbolt's and Park's, is a more involved matter. For these cases the overshoot characteristics of the starting procedure must be

ascertained and, in addition, the interaction between the multistep method and all possible data generated by the starting procedure must be evaluated.

5.2. Numerical Comparisons

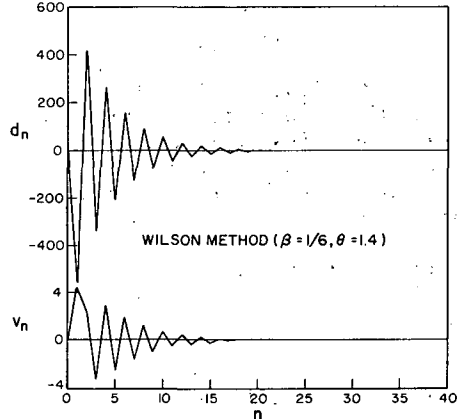
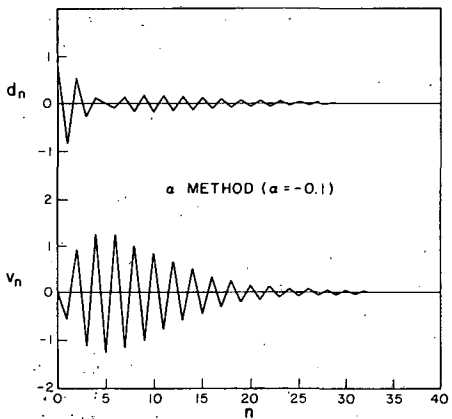
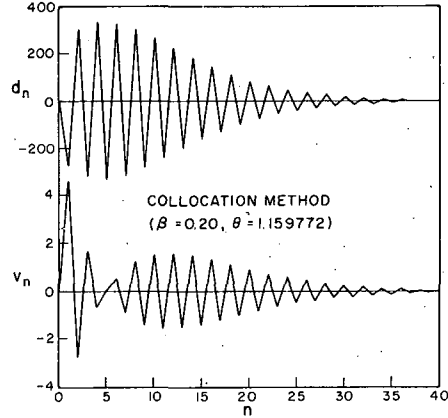
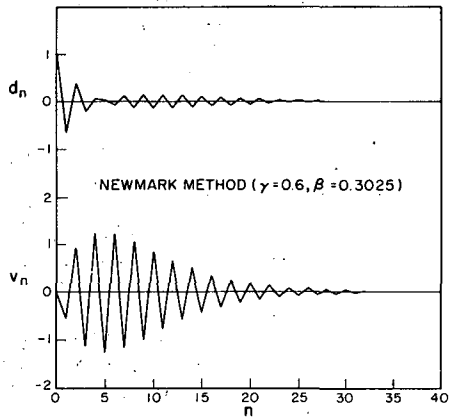
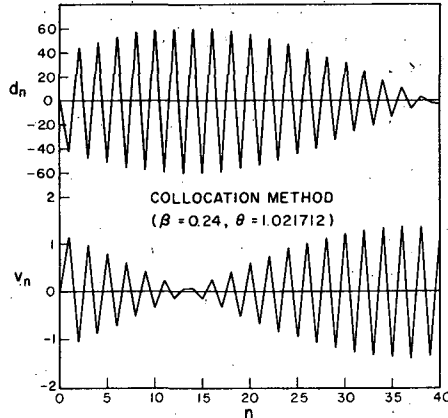
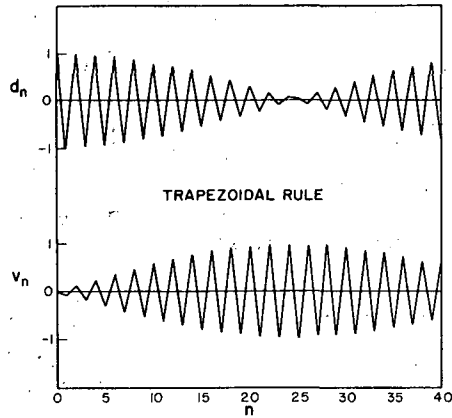
Since all the algorithms considered are convergent there can be no overshoot in the limit $\Omega \rightarrow 0$. Thus, in obtaining the following formulas we have assumed $\Omega \rightarrow \infty$. The solutions at the end of step 1, for the initial conditions (d,v), are given as follows:

Collocation schemes:

$$\left(\frac{\theta}{2(\theta + 1)} \geq \beta \geq \frac{2\theta^2 - 1}{4(2\theta^3 - 1)} \right), \quad \theta \geq 1$$

$$d_1 \approx -\frac{1}{2} \left(1 - \frac{1}{\theta} \right) \Omega^2 d + \left(1 - \frac{1}{\theta^2} \right) \Delta t v \quad (5.11)$$

$$v_1 \approx \left(\frac{1}{4\beta\theta} - 1 \right) \Omega \omega d + \left(1 - \frac{1}{2\beta\theta^2} \right) v \quad (5.12)$$



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Figure 9. Comparison of overshoot response for several methods.

α methods: ($\beta = (1 - \alpha)^2/4$, $\gamma = 1/2 - \alpha$, $\alpha \in [-1/3, 0]$)

$$d_1 \approx \left(1 - \frac{1}{2\beta(1 + \alpha)}\right) d \quad (5.13)$$

$$v_1 \approx \left(\frac{\gamma}{2\beta} - 1\right) \Omega \omega d + (1 - \gamma/\beta) v \quad (5.14)$$

Retaining only significant terms according to order of magnitude and assuming neither $\theta = 1$ nor $\alpha = 0$, we get:

Collocation schemes:

$$d_1 \sim 0(\Omega^2)d + 0(\Delta t)v \quad (5.15)$$

$$v_1 \sim 0(\Omega)\omega d + 0(1)v \quad (5.16)$$

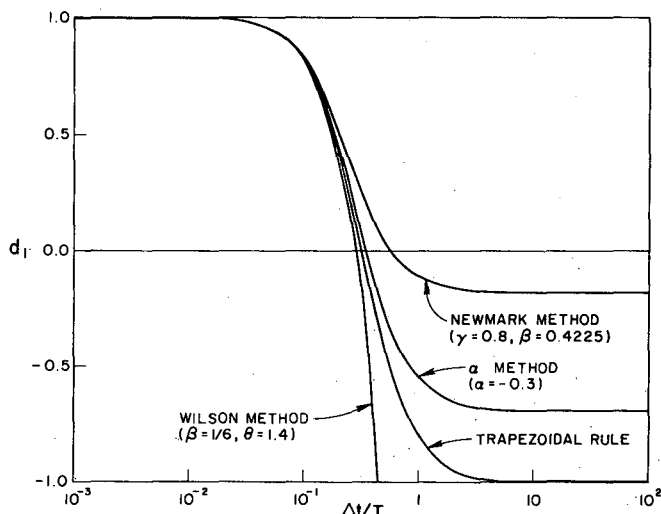
α methods:

$$d_1 \sim 0(1)d \quad (5.17)$$

$$v_1 \sim 0(\Omega)\omega d + 0(1)v \quad (5.18)$$

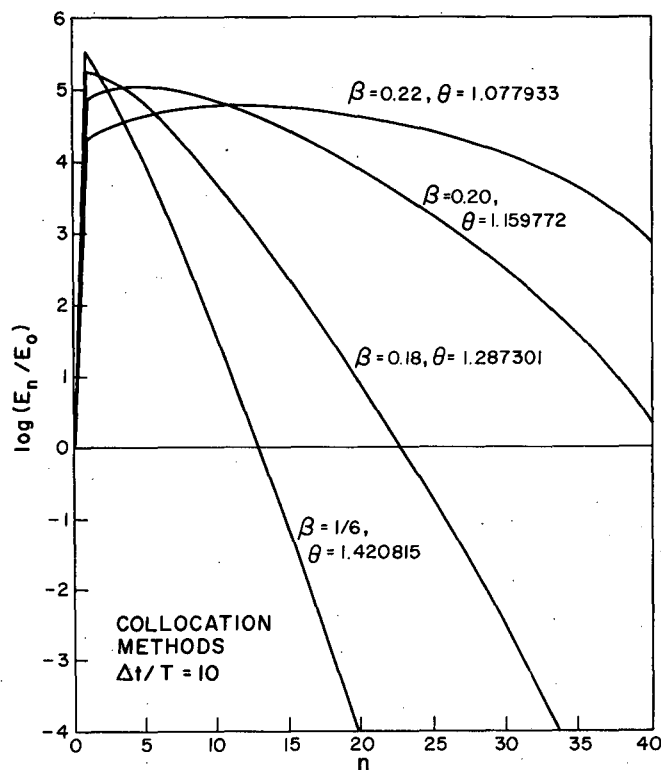
Both methods exhibit a tendency to overshoot linearly in Ω in the velocity equation due to the initial displacement terms. The α methods exhibit no overshoot in displacement. On the other hand, d_1 of the collocation schemes overshoots quadratically in Ω due to initial displacement, and linearly in Δt due to initial velocity. The superiority of the α methods over the collocation schemes with regard to overshoot is evident.

For both families the critical condition is caused by initial displacement. In Figure 9 numerical results for some of the present schemes are exhibited for initial data $d = 1$ and $v = 0$, and $\Delta t/T = 10$. The trapezoidal rule and representatives of the Newmark and Wilson methods are



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Figure 10. Displacement at end of first time step for several methods versus $\Delta t/T$.



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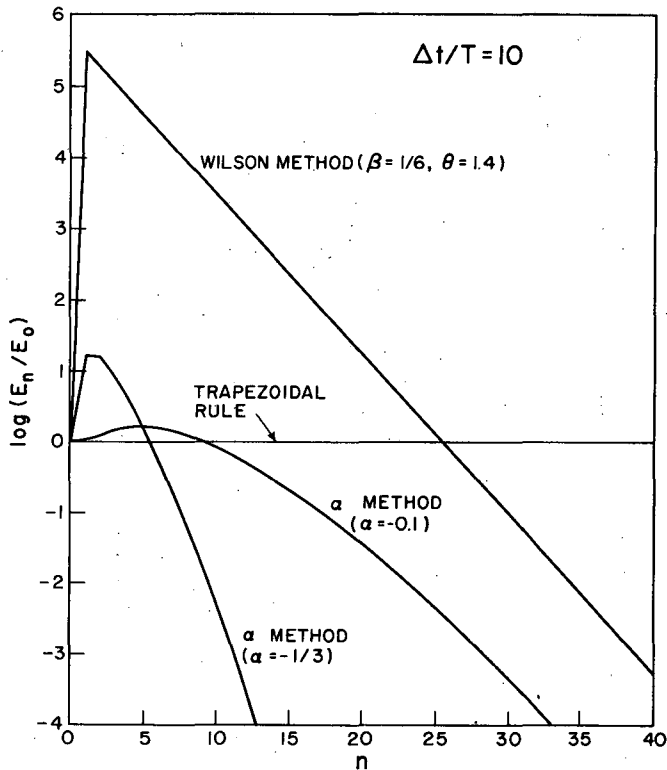
Figure 11. Energy overshoot response for optimal collocation schemes.

included for comparison purposes. The trapezoidal rule exhibits no overshoot in either the displacements or velocities. Mild overshooting is exhibited by the velocities in the Newmark and α methods, but none in displacements. The pathological displacement overshoot characteristics of two optimal collocation schemes and the Wilson method are manifest, whereas the velocities for these cases overshoot only mildly.

In Figure 10 the behavior of d_1 over the full range of Δt is presented for several methods.

Energy comparisons of optimal collocation schemes are presented in Figure 11 for the same initial value problem as previously considered. Note that for the higher values of β , the decay of the overshoot is extremely slow. The Wilson, trapezoidal, and α methods are compared in Figure 12. The overshoot of the α methods is due solely to the kinetic energy. As is well known the trapezoidal rule conserves energy for the problem at hand (see e.g. [2], [14] and [15]) and thus exhibits no overshoot.

The fact that the α method exhibits no overshoot in displacements, but overshoots linearly in velocity suggests that further improvement can be made simply by viewing the presently defined velocities as intermediate quantities, and using difference formulas to obtain the discrete velocities from the displacements.



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Figure 12. Comparison of energy overshoot response for several methods.

Conclusions

In this paper we have systematically generalized and analyzed the concept of collocation, originally used by Wilson in the development of second-order accurate, unconditionally stable, dissipative one-step methods in structural dynamics. Optimal schemes within this class have been developed and compared with the recently proposed family of α methods. The α methods are found to be superior with respect to standard measures of dissipation and dispersion.

It is argued that the tendency to overshoot is an important and independent factor which should be considered in an evaluation of an implicit scheme. A basis is established for studying overshoot and the optimal collocation and α methods are compared. It is found that pathological overshooting is an inherent property of collocation schemes, whereas the overshooting characteristics of the α methods are good.

Further research is justified in several areas. In linear analysis the interaction of the viscous damping term with the step-by-step integrator has yet to be seriously studied. There are indications that some delicate handling may be called for (see [5]). The α schemes should be tested in the nonlinear regime. The analysis of nonlinear algorithms has barely begun and controversy reigns (see [2,4,14,15,20]).

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