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Numerical Instability due to Varying Time Steps in Explicit Wave Propagation and Mechanics Calculations

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Explicit central-difference time integration is frequently used to solve the wave equation, and the classical criterion for numerical stability is the Courant–Friedrichs–Lewy condition. Similarly, explicit integration of a spring-mass mechanical system has a stability condition. These conditions are derived under the assumption of constant time steps. This paper demonstrates the new and perhaps surprising result that numerical instability may occur when time steps vary, even though all steps are substantially less than the constant step criterion.

INTRODUCTION

As discussed by Richtmyer and Morton [1, pp. 260–263], the usual finite-difference approximation for the one-dimensional wave equation $\partial^2 y/\partial t^2 = c^2(\partial^2 y/\partial x^2)$ is

$$y_j^{n+1} - 2y_j^n + y_j^{n-1} = \left(\frac{c\Delta t}{\Delta x}\right)^2 \left(y_{j+1}^n - 2y_j^n + y_{j-1}^n\right), \tag{1}$$

where c is the wave speed, Δx is the space interval, and Δt is the time step. If the Courant–Friedrichs–Lewy (CFL) condition, $c\Delta t/\Delta x < 1$, holds, method (1) is numerically stable. Otherwise, it is unstable. Interpreting (1) as a special case of a spring-mass system,

$$M\ddot{y} + Ky = 0, \tag{2}$$

yields the same result, as follows. First approximate the spatial derivative of the wave equation by central differences with constant spacing Δx. The mass matrix, M, is the identity matrix. The stiffness matrix, K, is $(c/\Delta x)^2$ times a tridiagonal matrix that has diagonal entries equal to 2 and entries above and below the diagonal equal to -1.

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Solution of the eigenvalue problem $(K - \omega^2 M)v = 0$ permits diagonalization of system (2), resulting in an uncoupled set of linear oscillators, $\ddot{z} + \omega^2 z = 0$. Thus analysis of the stability of a time integration method for the wave equation, or any spring-mass system, reduces to the study of a single undamped linear oscillator. If system (2) is integrated with the explicit central-difference method, numerical stability requires

$$\Delta t < 2/\omega_{\max}, \tag{3}$$

where $\omega_{\max}$ is the maximum system frequency [2, p. 204]. For the wave equation treated as a lumped mass system, $\omega_{\max} = 2c/\Delta x$ [3, p. 102], which with (3) leads to the CFL condition. The preceding results are well established for constant time steps. Varying steps are discussed below.

CENTRAL DIFFERENCE METHOD WITH VARYING TIME STEPS

Consider the linear oscillator $\ddot{u} + u = 0$, where $u(\tau)$ is a function of the scaled time $\tau = \omega_{\max} t$. Explicit central-difference time integration, written as a one-step algorithm, corresponds to Newmark's method with $\beta = 0$ and $\gamma = 1/2$ [3, p. 82],

$$\begin{aligned} u_{n+1} &= u_n + p\dot{u}_n + p^2\ddot{u}_n/2 \\ \dot{u}_{n+1} &= \dot{u}_n + p(\ddot{u}_n + \ddot{u}_{n+1})/2, \end{aligned} \tag{4}$$

where the time step is $p = \tau_{n+1} - \tau_n > 0$. With the differential equation, $\ddot{u}_n = -u_n$, and some algebra, (4) becomes

$$\begin{bmatrix} u_{n+1} \\ \dot{u}_{n+1} \end{bmatrix} = G(p)\begin{bmatrix} u_n \\ \dot{u}_n \end{bmatrix} \equiv \begin{bmatrix} 1 - p^2/2 & p \\ -p + p^3/4 & 1 - p^2/2 \end{bmatrix}\begin{bmatrix} u_n \\ \dot{u}_n \end{bmatrix}. \tag{5}$$

The amplification matrix, $G(p)$, has the characteristic equation

$$\det[G(p) - \lambda I] = \lambda^2 - (2 - p^2)\lambda + 1 = 0. \tag{6}$$

If $p^2 \leq 4$, the roots of (6) satisfy $|\lambda| = 1$. For $p = 2$, there is a weak numerical instability associated with the double root, $\lambda = -1$ [1, p. 263]. Therefore, numerical stability requires $p < 2$. This result, which is the same as condition (3), holds when the time step is constant.

Now consider two different time steps in sequence, p then q, both satisfying the constant step criterion, $p < 2,\ q < 2$. The amplification matrix is the product $G(q)\,G(p)$, which has the characteristic equation

$$\lambda^2 - [2 - f_2(p, q)]\lambda + 1 = 0, \tag{7a}$$

where

$$f_2(p, q) = (p + q)^2(1 - pq/4). \tag{7b}$$

In the same way as for (6), numerical stability requires $f_2 < 4$. Hence, $f_2(p, q)$ is called the two-step stability function. Figure 1 shows the p-q plane with two curves corresponding to

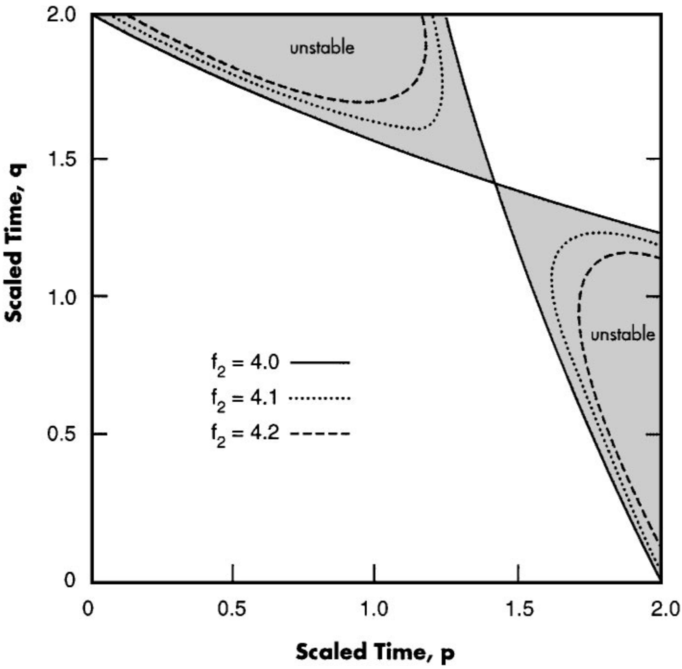

FIG. 1. Regions of instability defined by contours of the two-step stability function $f_2(p, q)$. Bifurcation point of f_2 is at $p = q = \sqrt{2}$.

$f_2 = 4$. These curves intersect at $p = q = \sqrt{2}$ and border two regions that contain contours corresponding to $f_2 = 4.1$ and 4.2. The stability function violates $f_2 < 4$ for all pairs of time steps inside these two regions. For example, $f_2(1.3, 1.5) = 4.018$. Therefore, if time steps alternate in the pattern 1.3, 1.5, 1.3, 1.5, ..., method (5) is unstable. This is illustrated in Fig. 2 which shows computed displacements, u_n, for the test problem $\ddot{u} + u = 0$, $u(0) = 1$, $\dot{u}(0) = 0$, integrated to $\tau_{100} = 140$ by calculating 50 repetitions with $p = 1.3$, $q = 1.5$. (Although the displacements appear to be zero at early times in Fig. 2, they are in fact nonzero.)

Other examples of instability are readily found by choosing pairs of time steps from within the regions of instability in Fig. 1. For example, Fig. 3 shows displacements when the test problem is integrated, to essentially the same final time as before, by doing ten repetitions with the following sequence of 10 time steps: 1.3, 1.5, 1.33, 1.45, 1.32, 1.47, 1.34, 1.48, 1.31, 1.46.

The intersection point in Fig. 1 at $p = q = \sqrt{2}$ is a bifurcation point of $f_2(p, q)$ in the following sense. Note that $f_2(p + \varepsilon, p - \varepsilon) = p^2(4 - p^2) + \varepsilon^2 p^2$. Therefore, $f_2(\sqrt{2} + \varepsilon, \sqrt{2} - \varepsilon) = 4 + 2\varepsilon^2$, which exceeds 4 for $\varepsilon \neq 0$. In other words, the root(s) of the polynomial $g_2(p) = f_2(p, p) - 4$ are possible bifurcation point(s) of the stability function. From (7b), $g_2(p) = p^2(4 - p^2) - 4 = -(p^2 - 2)^2$, which leads to the bifurcation point at $p = \sqrt{2}$.

Consider three time steps, p then q then r. The amplification matrix is the triple matrix product $G(r)G(q)G(p)$, which has the characteristic equation

$$\lambda^2 - [2 - f_3(p, q, r)]\lambda + 1 = 0, \tag{8a}$$

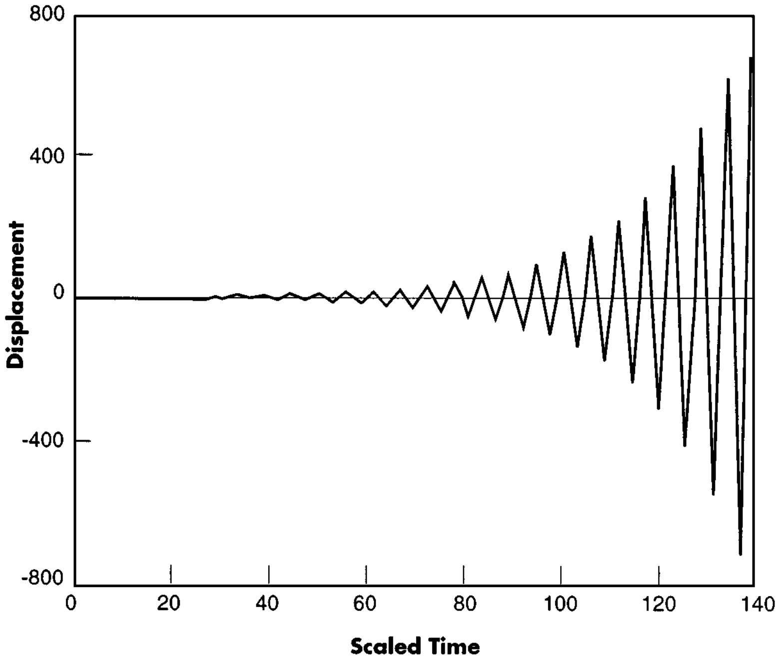

FIG. 2. Calculated displacements for $\ddot{u} + u = 0$, $u(0) = 1$, $\dot{u}(0) = 0$, integrated with the two-step pattern 1.3, 1.5.

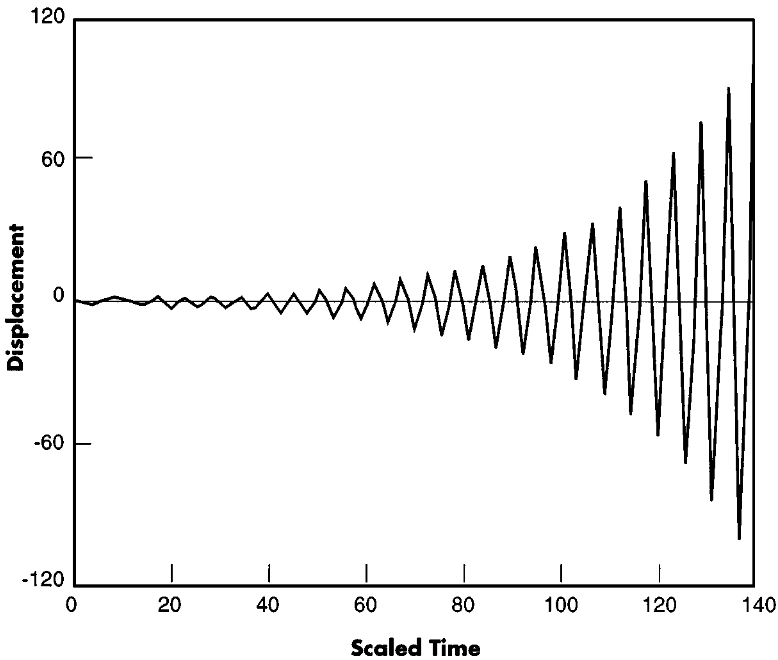

FIG. 3. Calculated displacements for $\ddot{u} + u = 0$, $u(0) = 1$, $\dot{u}(0) = 0$, integrated with the ten-step pattern 1.3, 1.5, 1.33, 1.45, 1.32, 1.47, 1.34, 1.48, 1.31, 1.46.

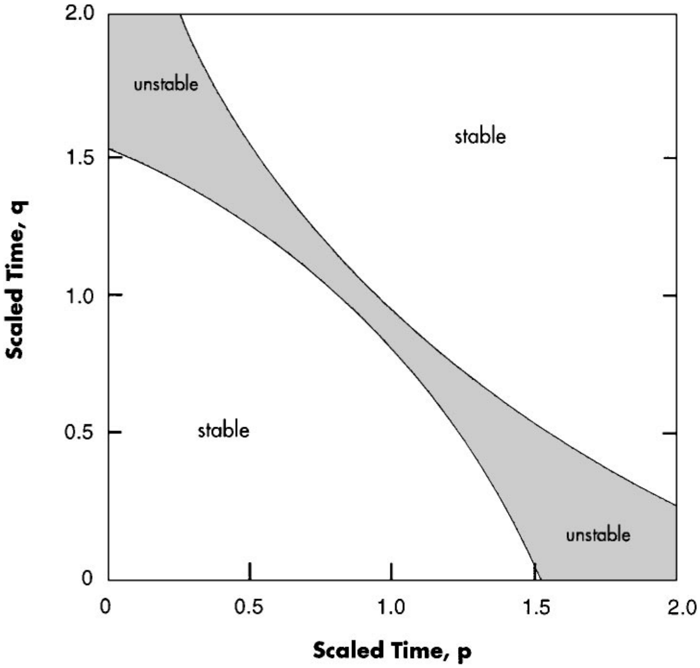

FIG. 4. A region of instability defined by two contours of the three-step stability function $f_3(p, q, 1.1) = 4$.

where

$$f_3(p,q,r) = (p+q+r)^2 - \frac{pq}{4}(p+q)^2 - \frac{qr}{4}(q+r)^2 - \frac{pr}{4}(p+r)^2 \\ -pqr(p+q+r) + \frac{pqr}{24}[(p+q+r)^3 - (p^3+q^3+r^3)]. \tag{8b}$$

The three-step stability function violates $f_3 < 4$ in various regions of p-q-r space. For example, Fig. 4 shows a region of instability defined by two curves corresponding to $f_3(p, q, 1.1) = 4$. Figure 5 shows results for the test problem integrated with $p = 0.9$, $q = 1, r = 1.1$.

It should be noted that, even though $f_2(p, q)$ and $f_3(p, q, r)$ are invariant with respect to the interchange of two variables, the amplification matrix is not, because $G(p)$ and $G(q)$ do not commute for $p \neq q$. Consequently, the order of time steps is important. Figure 6 shows results for 47 repetitions with $p = 1.1,\ q = 1,\ r = 0.9$. The differences between Figs. 5 and 6 are due to the reversed time steps (although the real culprit is instability due to varying time steps). The differences appear because, in a region of instability, both roots of the characteristic polynomial are real and negative, with one satisfying $|\lambda| > 1$ and the other $|\lambda| < 1$. For a series of unstable time steps, the early-time results depend on the phasing of the initial displacement and velocity. However, after many steps, the root of larger magnitude will dominate, reflecting the inherent instability. If, instead, three time steps are chosen from a stable region, exponential growth cannot occur and the results are much less sensitive to time step order. For example, regardless of whether the test problem is integrated for many hundreds of steps with the three-step pattern 1.0, 0.9, 0.8 or its reverse, 0.8, 0.9, 1.0, the displacements oscillate between -1.054 and $+1.054$.

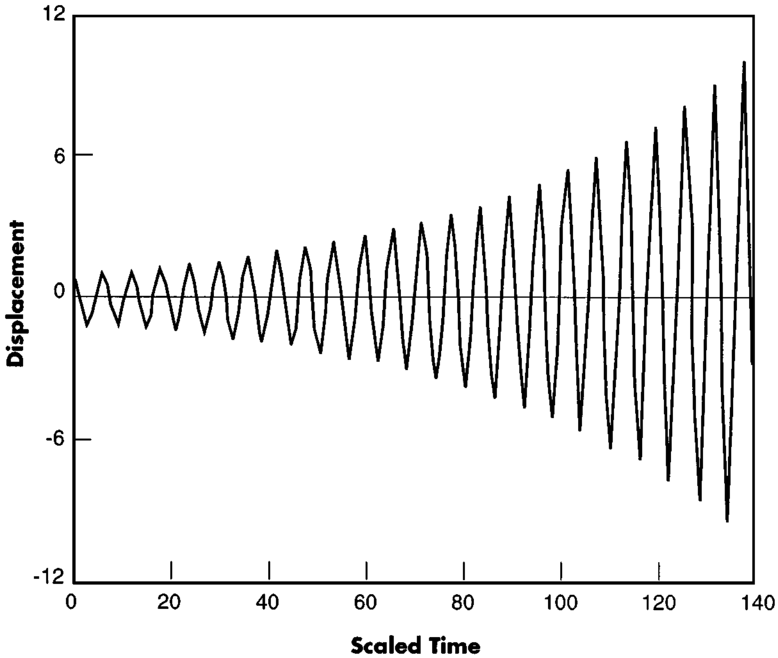

FIG. 5. Calculated displacements for $\ddot{u} + u = 0$, $u(0) = 1$, $\dot{u}(0) = 0$, integrated with the three-step pattern 0.9, 1.0, 1.1 (see Fig. 6).

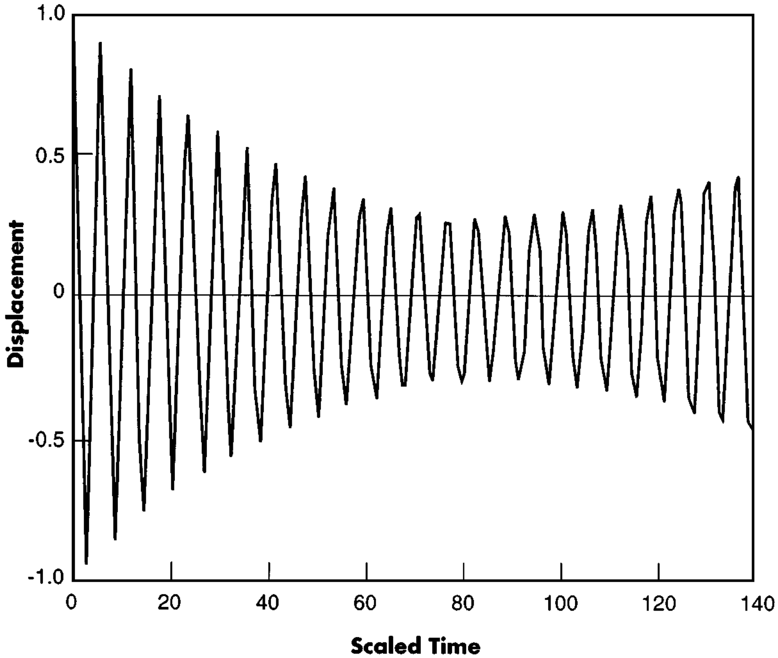

FIG. 6. Calculated displacements for $\ddot{u} + u = 0$, $u(0) = 1$, $\dot{u}(0) = 0$, integrated with the three-step pattern 1.1, 1.0, 0.9 (see Fig. 5).

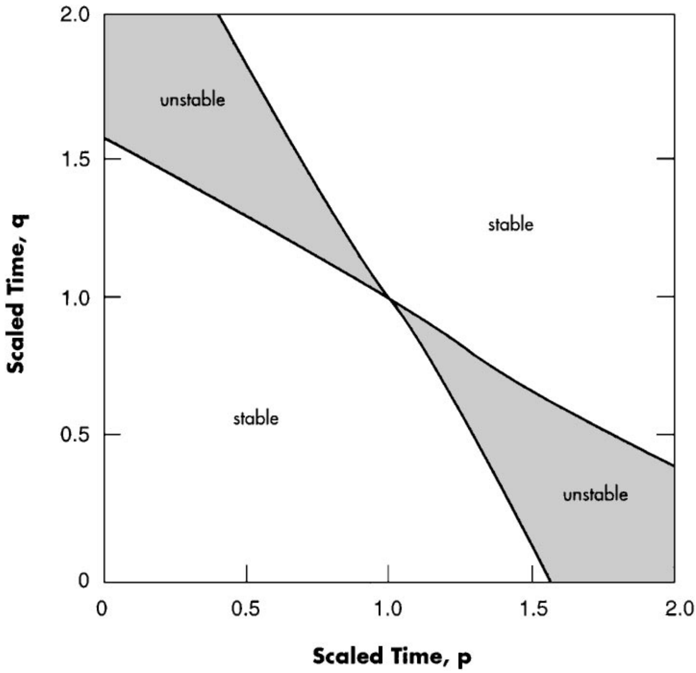

FIG. 7. Regions of instability defined by two contours of $f_3(p, q, 1) = 4$. Bifurcation point of f_3 is at $p = q = r = 1$.

The three-step bifurcation polynomial is $g_3(p) = f_3(p, p, p) - 4 = p^6 - 6p^4 + 9p^2 - 4 = (p^2 - 4)(p^2 - 1)^2$. Thus $p = 1$ is a bifurcation point satisfying $0 < p < 2$. Figure 7 shows $f_3(p, q, 1) = 4$ and two regions of instability. Note that Fig. 4 does not have a bifurcation point; instead, there are two curves defining a single region of instability.

The stability functions, being polynomials in several variables, are continuous. Because $f_3(p, q, 0) = f_2(p, q)$, it is clear that, as r increases from zero, the regions of instability of f_3, defined by surfaces in p-q-r space, are connected continuously to those of f_2 in the p-q plane.

The preceding results generalize as follows. Consider n steps in sequence, $p, q, r, \ldots$. The n-step amplification matrix has a second-degree characteristic equation, as in (7a) and (8a). The n-step stability function $f_n(p, q, r, \ldots)$ is a polynomial in several variables, continuously connected to f_{n-1}; from (6), $f_1(p) \equiv p^2$. Regions of stability and instability are separated in n-dimensional hyperspace by hypersurfaces corresponding to $f_n = 4$. The bifurcation function, $g_n(p) = f_n(p, p, p, \ldots) - 4$, is a polynomial of degree n in p^2. Table 1 lists the bifurcation points for $2 \leq n \leq 6$. Note that these points decrease as n increases; no lower bound on bifurcation points has been found.

As a final example, Fig. 8 shows a region of instability defined by $f_6(p, q, 0.3, 0.4, 0.5, 0.6) = 4$. Figure 9 shows results for the test problem integrated with the six-step pattern 0.3, 0.4, 0.5, 0.5, 0.6, 0.8. Although the exponential rate of growth is slower than in previous examples, instability is still evident.

CLOSURE

The preceding examples may seem to be abstract pathological instabilities of no real concern but it was just such an instability that stimulated this study [4]. The instability

TABLE 1
Bifurcation Points of the *n*-Step Stability Function

n	Bifurcation point
2	$\sqrt{2} \cong 1.41$
3	1
4	$\sqrt{2-\sqrt{2}} \cong 0.765$
5	$(\sqrt{5}-1)/2 \cong 0.618$
6	$\sqrt{2-\sqrt{3}} \cong 0.518$

occurred during a short part of a nonlinear calculation where time steps alternated in size by roughly a factor of two; that is, Δt, $\Delta t/2$, Δt, $\Delta t/2, \ldots$. This pattern persisted for 67 time steps and then stopped. Erroneous results appeared later in the calculation.

The new variable-step instability identified here may help to explain previously unexplained numerical difficulties (e.g., see "arrested stability" in [5, p. 50]). Constant time steps are usually assumed when doing numerical stability analyses, and constant steps are normally used when solving linear problems. However, in nonlinear computations, time steps are typically varied below some threshold determined by a constant step criterion. The above analysis, based on linear theory, shows that varying time steps may be a source of numerical instability and, hence, inaccurate results. Nonlinearities may obscure these errors

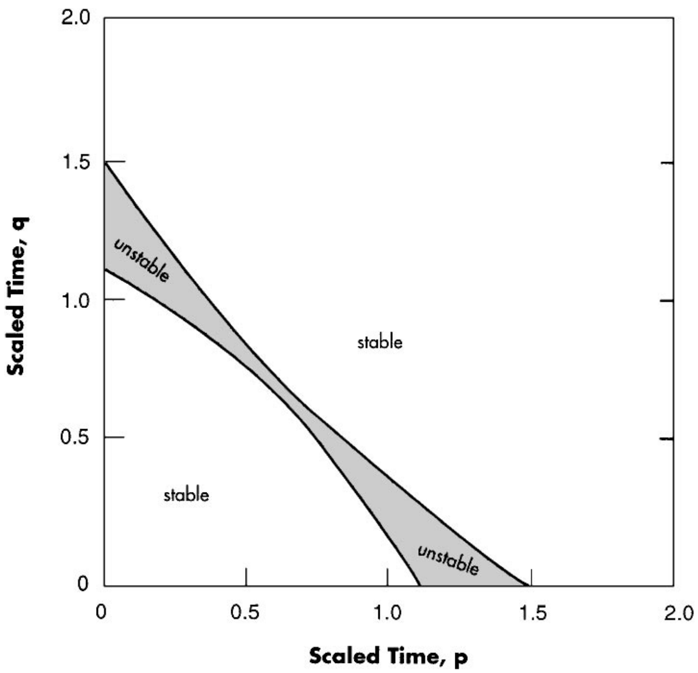

FIG. 8. A region of instability defined by two contours of $f_6(p, q, 0.3, 0.4, 0.5, 0.6) = 4$. Bifurcation point of f_6 is at $p = q = r = \cdots = \sqrt{2-\sqrt{3}} \cong 0.518$.

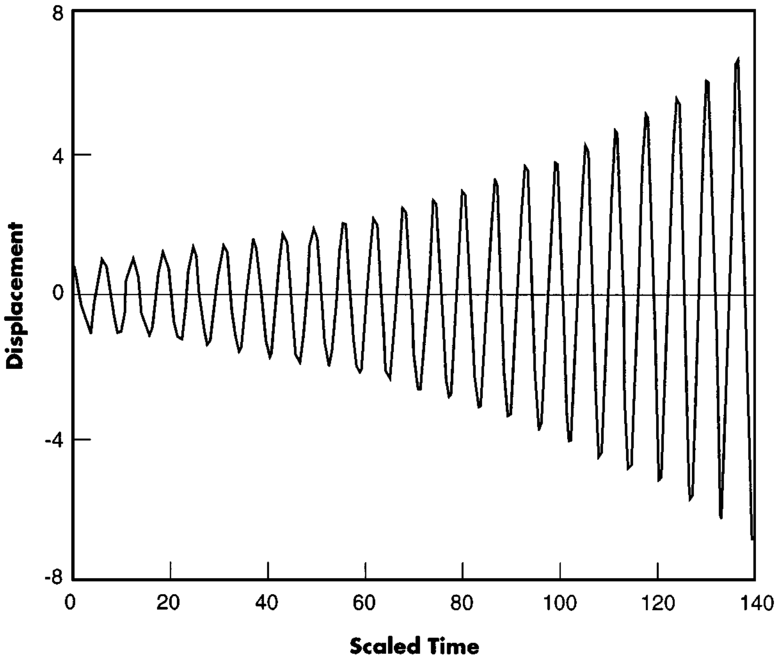

FIG. 9. Calculated displacements for $\ddot{u} + u = 0$, $u(0) = 1$, $\dot{u}(0) = 0$, integrated with the six-step pattern 0.3, 0.4, 0.5, 0.5, 0.6, 0.8.

but they cannot eliminate them. It is worth noting that integrating a variable-stiffness system with constant time steps resembles integrating a constant-stiffness system with varying time steps.

The speed and capacity of computers continue to increase rapidly, and highly complex computations are now commonplace. These computations often involve either adaptive mesh techniques (where elements are either subdivided or combined and time steps are changed accordingly) or subcycling (where different elements have different and varying time steps based on material state) or both. The likelihood of encountering variable-step instabilities can only increase in the future. What is needed are methods that avoid variable-step instabilities but have the efficiency of the central difference method. Some unconditionally stable implicit methods may have the first attribute. It is well known that they do not have the second. Implicit–explicit methods have the potential for both. Research in this direction is in progress (see Appendix).

APPENDIX A: AVOIDING VARIABLE-STEP INSTABILITIES

This appendix summarizes some results and ideas on methods for avoiding variable-step instabilities. So far, no satisfactory alternative has been found to the explicit central difference method for solving nonlinear mechanics problems.

Consider the unconditionally stable Newmark method with $\beta = 1/2$ and $\gamma = 1/2$,

$$\begin{aligned} u_{n+1} &= u_n + p\dot{u}_n + p^2\ddot{u}_{n+1}/2 \\ \dot{u}_{n+1} &= \dot{u}_n + p(\ddot{u}_n + \ddot{u}_{n+1})/2, \end{aligned} \tag{A.1}$$

where the time step is $p = \tau_{n+1} - \tau_n > 0$. With the differential equation, $\ddot{u}_n = -u_n$, and some algebra, (A.1) becomes

$$\begin{bmatrix} u_{n+1} \\ \dot{u}_{n+1} \end{bmatrix} = H(p) \begin{bmatrix} u_n \\ \dot{u}_n \end{bmatrix} \equiv \frac{1}{1+p^2/2} \begin{bmatrix} 1 & p \\ -p-p^3/4 & 1 \end{bmatrix} \begin{bmatrix} u_n \\ \dot{u}_n \end{bmatrix}. \tag{A.2}$$

The amplification matrix, $H(p)$, has the characteristic equation

$$\det[H(p) - \lambda I] = \lambda^2 - [2 - h_1(p)]\lambda + 1 = 0, \tag{A.3}$$

where

$$h_1(p) = \frac{p^2}{1+p^2/2}. \tag{A.4}$$

The one-step stability function, h_1, satisfies the stability condition $h_1 < 4$ for any time step $p > 0$, which it must since the method is unconditionally stable.

Consider two time steps in sequence, p then q. The amplification matrix, $H(q)H(p)$, has the characteristic equation

$$\lambda^2 - [2 - h_2(p,q)]\lambda + 1 = 0, \tag{A.5}$$

where

$$h_2(p,q) = \frac{(p+q)^2(1+pq/4)}{(1+p^2/2)(1+q^2/2)}. \tag{A.6}$$

Study of (A.6) shows that the stability condition, $h_2 < 4$, is satisfied if $p < 2, q < 2$, the limit of the explicit central difference method. This is acceptable since it shows that (A.1) prevents two-step instabilities for time steps of interest in wave propagation calculations. It is conjectured that (A.1) would have prevented the two-step instability associated with alternating time steps, $\Delta t, \Delta t/2, \Delta t, \Delta t/2, \ldots$, mentioned in the Closure. One way to check this would be to implement (A.1) instead of the explicit central difference method. This means implementing an implicit method which is quite inefficient compared to the explicit method. Alternatives such as implicit–explicit (also called partitioned or semi-implicit) methods might then be explored. However, before pursuing this path, it is prudent to look for n-step instabilities of (A.1) for higher n.

Instead of deriving analytic expressions for higher n, it is simpler to do numerical searches by computing the stability function $h_n(p,q,r,\ldots)$ from $h_n = 2 - \operatorname{trace}(A_n)$, where A_n is the amplification matrix $A_n(p,q,r,\ldots) = \ldots H(r)\,H(q)\,H(p)$. Doing this for (A.1) shows that the three-step stability function has a bifurcation point at $p = q = r = \sqrt{2}$. Contour plots of $h_3(p,q,\sqrt{2})$ confirm this. Thus (A.1) has three-step instabilities for time steps of interest in wave propagation calculations, an unsatisfactory result. It therefore seems likely that bifurcation points exist at smaller time steps for higher n, although this has not been confirmed.

What seems desirable is a method that prevents n-step instabilities for all n. Consider the following unconditionally stable method based on the exact solution of $\ddot{u} + u = 0$,

$$\begin{bmatrix} u_{n+1} \\ \dot{u}_{n+1} \end{bmatrix} = E(p) \begin{bmatrix} u_n \\ \dot{u}_n \end{bmatrix} \equiv \begin{bmatrix} \cos p & \sin p \\ -\sin p & \cos p \end{bmatrix} \begin{bmatrix} u_n \\ \dot{u}_n \end{bmatrix}. \tag{A.7}$$

The one-step stability function of (A.7) is $e_1(p) = 2 - \text{trace}(E(p)) = 2(1 - \cos p)$, which satisfies $e_1 < 4$ for all p (except odd multiples of π which cannot cause weak instabilities since (A.7) is exact). The two-step amplification matrix is $E(q)E(p)$ which equals $E(p+q)$ by trigonometric identities. This can be extended by induction for any number of time steps and it is simple to show that (A.7) is unconditionally stable with respect to time step variations for any number of time steps, as would expected since (A.7) is based on the exact solution. Ways are being explored to extend (A.7) to more than one degree of freedom and, then, to an efficient method for nonlinear systems.

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