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Stability and Accuracy of Differencing Methods for Viscoplastic Models in Wavecodes

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The numerical stability and truncation error of a family of differencing schemes for viscoplastic constitutive relations in wavecodes is investigated. A von Neumann stability analysis is performed for a one-dimensional model problem. This analysis identifies two differencing methods that have no restriction on the time step size beyond the usual Courant–Friedrichs–Lewy condition. One of these methods is first-order accurate, and the other is second-order accurate. Implementation of one of these methods in the three-dimensional wavecode CTH is discussed.

1. INTRODUCTION

Viscoplastic models are finding increasing use in wavecodes as analysts require improved accuracy in computing the strengths of ductile metals under a wide range of conditions of temperature and strain rate. Well-known models for the viscoplastic response of metals include those of Johnson and Cook [1], Zerilli and Armstrong [2], Follansbee and co-workers [3], and Steinberg and co-workers [4, 5].

Code developers attempting to install models of this type in wavecodes have informally reported problems with numerical instability. This was also the author's experience when installing the Johnson–Cook and Zerilli–Armstrong models in CTH [6], an Eulerian wavecode.

In order to investigate the source of this instability in a simpler setting, the author wrote a small, one-dimensional Lagrangian wavecode employing the Johnson–Cook model. The differencing scheme was the method referred to as "backward-explicit" described in Section 2 of this paper. Numerical noise occurred even in this simple Lagrangian model, suggesting that the source of the problem was not some feature of the Eulerian remap scheme in CTH. The noise remained even when a very small time step was used.

To gain a better understanding of why the noise occurred, a von Neumann stability analysis was performed for a family of differencing schemes. The analysis showed that the backward-explicit method is unstable. However, it also showed that among this family of methods, two involved no stability restriction on the time step beyond the usual Courant–Friedrichs–Lewy (CFL) condition. These methods are referred to below as the "backward-implicit" and "three-point" methods. Although these approaches are implicit, they do not require the solution of a large set of linear equations, and they can be integrated into a wavecode without undue difficulty. The purpose of this paper is to report the results of this analysis and to describe implementation of the backward-implicit approach in CTH.

2. DIFFERENTIAL EQUATIONS AND DIFFERENCE FORMULAS

The system of partial differential equations to be analyzed is a one-dimensional model of the dynamics of a homogeneous viscoplastic solid under conditions of uniaxial strain. We start from the full three-dimensional system of equations and specialize it to uniaxial strain below. In the following, x_i is position, t is time, ρ is density, u_i is displacement, σ_{ij} is the Cauchy stress tensor, and ε_{ij} is the linearized strain tensor. Material isotropy and small displacement gradients are assumed. The equation of motion and the displacement–strain relation are

$$\rho \ddot{u}_i = \sigma_{ij,j} \tag{1}$$

$$\varepsilon_{ij} = \tfrac{1}{2}(u_{i,j} + u_{j,i}), \tag{2}$$

where the notation for partial derivatives is $(\dot{}) = \partial(\ )/\partial t$ and $(\ )_{,j} = \partial(\ )/\partial x_j$. The deviatoric strain is

$$e_{ij} = \varepsilon_{ij} - \vartheta \delta_{ij}/3, \tag{3}$$

where ϑ is the dilatation,

$$\vartheta = \varepsilon_{kk}. \tag{4}$$

Making the usual assumption for an elastic–plastic solid,

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the deviatoric strain rate tensor is decomposed into elastic and plastic parts:

$$\dot{e}_{ij} = \dot{e}^{\mathrm{e}}_{ij} + \dot{e}^{\mathrm{p}}_{ij}. \tag{5}$$

The stress tensor is computed as

$$\sigma_{ij} = k\vartheta\delta_{ij} + S_{ij}, \tag{6}$$

where k is the bulk modulus and S_{ij} is the deviatoric stress tensor, found from

$$\dot{S}_{ij} = 2\mu\dot{e}^{\mathrm{e}}_{ij}, \tag{7}$$

where μ is the shear modulus. Because of plastic flow, the deviatoric stress tensor is constrained to lie within or on the yield surface:

$$|\mathbf{S}| \equiv \sqrt{S_{ij}S_{ij}} \leqslant \sqrt{2/3}\, Y, \tag{8}$$

where Y is the yield stress. After yielding, the plastic part of the strain rate tensor is determined by the flow rule

$$\dot{e}^{\mathrm{p}}_{ij} = \begin{cases} 0, & |\mathbf{S}| < \sqrt{2/3}\, Y \\ \lambda S_{ij}, & |\mathbf{S}| = \sqrt{2/3}\, Y, \end{cases} \tag{9}$$

where λ is some nonnegative number. λ must be nonnegative because plastic flow cannot occur in a direction opposite to the stress tensor that induces it. The determination of the yield stress is discussed next.

For a viscoplastic solid we assume that the yield stress is given by a function of the form

$$Y = Y(T, \varepsilon^{\mathrm{p}}, \dot{\varepsilon}^{\mathrm{p}}), \tag{10}$$

where T is the temperature and ε^{p} is the equivalent plastic strain, defined through its time derivative by

$$\dot{\varepsilon}^{\mathrm{p}} = \sqrt{\tfrac{2}{3}\dot{e}^{\mathrm{p}}_{ij}\dot{e}^{\mathrm{p}}_{ij}}. \tag{11}$$

For example, the Johnson–Cook model [1] has the form

$$Y = (A + B\varepsilon^{\mathrm{p}N})(1 + C\ln(\max(0.002, \dot{\varepsilon}^{\mathrm{p}}))) \times (1 - \theta^m), \tag{12}$$

where A, B, C, m, and N are positive constants, the units of $\dot{\varepsilon}^{\mathrm{p}}$ are s^{-1}, and θ is the homologous temperature, defined by

$$\theta = \frac{T - T_{\mathrm{r}}}{T_{\mathrm{M}} - T_{\mathrm{r}}}, \tag{13}$$

in which T_{r} is room temperature and T_{M} is the melting temperature of the material.

We now specialize the above system of equations to the case of uniaxial strain. We assume that

$$u_1 = u_1(x_1, t) \qquad u_2 = u_3 = \partial/\partial x_2 = \partial/\partial x_3 = 0. \tag{14}$$

The equation of motion (1) becomes

$$\rho\ddot{u}_1 = \sigma_{11,1}. \tag{15}$$

It follows from (2) that

$$[\varepsilon_{ij}] = \begin{pmatrix} u_{1,1} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{16}$$

From (16), (4), and (3),

$$[e_{ij}] = \begin{pmatrix} 2u_{1,1}/3 & 0 & 0 \\ 0 & -u_{1,1}/3 & 0 \\ 0 & 0 & -u_{1,1}/3 \end{pmatrix} \tag{17}$$

and

$$\vartheta = u_{1,1}. \tag{18}$$

The deviatoric strain rate decomposition (5) implies

$$\dot{e}_{11} = \dot{e}^{\mathrm{e}}_{11} + \dot{e}^{\mathrm{p}}_{11}. \tag{19}$$

From isotropy and the symmetry of the problem we see that the most general form of the deviatoric stress tensor in uniaxial strain is

$$[S_{ij}] = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & -S_{11}/2 & 0 \\ 0 & 0 & -S_{11}/2 \end{pmatrix}. \tag{20}$$

From (6), (18), and (20), the axial component of stress is

$$\sigma_{11} = ku_{1,1} + S_{11}. \tag{21}$$

Combining (8) with (20) results in the following condition:

$$-2Y/3 \leqslant S_{11} \leqslant 2Y/3. \tag{22}$$

The flow rule (9), together with (22) and (7), results in the specialized form of the constitutive law:

$$\dot{S}_{11} = 2\mu\dot{e}^{\mathrm{e}}_{11}, \tag{23}$$

$$\dot{e}^{\mathrm{p}}_{11} = \begin{cases} 0, & |S_{11}| < 2Y/3 \\ \lambda\,\mathrm{sgn}(S_{11}), & |S_{11}| = 2Y/3, \end{cases} \tag{24}$$

where λ is a nonnegative number.

The viscoplastic constitutive model (10) is unchanged by the assumption of uniaxial strain. However, under this assumption (11) can be simplified as follows: Note that the most general form of the plastic strain rate tensor is

$$[\dot{e}^{\mathrm{p}}_{ij}] = \begin{pmatrix} \dot{e}^{\mathrm{p}}_{11} & 0 & 0 \\ 0 & -\dot{e}^{\mathrm{p}}_{11}/2 & 0 \\ 0 & 0 & -\dot{e}^{\mathrm{p}}_{11}/2 \end{pmatrix} \tag{25}$$

because this tensor is deviatoric. Hence (11) becomes

$$\dot{\varepsilon}^{\mathrm{p}} = \dot{e}^{\mathrm{p}}_{11}. \tag{26}$$

Our objective is to define a one-dimensional model problem that will give insight into the stability issues that would arise in a multidimensional wavecode. We assume that a small displacement field w_1 is superposed on a homogeneous, steady stretching deformation

$$u_1(x_1, t) = \alpha x_1 t + w_1(x_1, t), \tag{27}$$

where α is a small positive number and w_1 is a function such that $|\dot{w}_{1,1}| < \alpha$. This ensures that

$$\dot{e}_{11} > 0. \tag{28}$$

We further assume that the body is yielded and in tension at all times:

$$S_{11} = 2Y/3. \tag{29}$$

This means that we do not need to worry about the absolute value signs in (24).

It was assumed in the derivation of the partial differential equations above that all displacement gradients are small. Therefore no further linearization of the kinematic equations or the equation of motion is necessary. However, it is necessary to linearize the constitutive law.

The dependence of Y on its first and second arguments is ignored in the following analysis, because in practice Y is a slowly varying function of these quantities and they have no practical effect on numerical stability. We can linearize the yield stress in the viscoplastic model (10) about the plastic strain rate $2\alpha/3$, for if $w_1 \equiv 0$, then by (17), $\dot{e}^{\mathrm{p}}_{11} = 2\alpha/3$ everywhere. The linearization is

$$Y = Y_0 + b(\dot{e}^{\mathrm{p}}_{11} - 2\alpha/3), \tag{30}$$

where Y_0 and b are constants defined by

$$Y_0 = Y(T, \varepsilon^{\mathrm{p}}, 2\alpha/3), \qquad b = \frac{\partial Y}{\partial \dot{\varepsilon}^{\mathrm{p}}}(T, \varepsilon^{\mathrm{p}}, 2\alpha/3). \tag{31}$$

In defining difference equations for the model problem, the objective is to emulate the way a typical multidimensional wavecode would work. Therefore we ignore the obvious simplifications that could be made in the system of differential equations for the model problem prior to writing the difference equations.

We first summarize the field equations to be differenced. The following substitutions are made in order to simplify the notation:

$$\begin{aligned} &x = x_1, \quad u = u_1, \quad w = w_1, \quad \sigma = \sigma_{11}, \\ &e = e_{11}, \quad e^{\mathrm{e}} = e^{\mathrm{e}}_{11}, \quad e^{\mathrm{p}} = e^{\mathrm{p}}_{11}. \end{aligned} \tag{32}$$

Also, the notation $(\ )_x = \partial(\ )/\partial x$ will be used. Using (27), the equation of motion (15) is

$$\rho \ddot{w} = \sigma_x. \tag{33}$$

From (21), (27), and (29),

$$\sigma = k(\alpha t + w_x) + 2Y/3. \tag{34}$$

From (17) and (27),

$$\dot{e} = \tfrac{2}{3}(\alpha + \dot{w}_x). \tag{35}$$

From (19),

$$\dot{e} = \dot{e}^{\mathrm{e}} + \dot{e}^{\mathrm{p}}. \tag{36}$$

From (29) and (23),

$$\dot{e}^{\mathrm{e}} = \dot{Y}/3\mu. \tag{37}$$

From (30),

$$Y = Y_0 + b(\dot{e}^{\mathrm{p}} - 2\alpha/3). \tag{38}$$

In the following discussion, discretized quantities will be represented in the form $\phi_{j,n}$, where j is the spatial index, $-\infty < j < \infty$, and n is the time step index, $0 \leqslant n < \infty$. The zone size Δx and time step length Δt are assumed to be constant. The variables σ, e, e^{p}, and e^{e} are zone-centered quantities, while w and its time derivatives are node-centered. Differences will be abbreviated using the notation

$$\begin{aligned} (\delta_x \phi)_{j+1/2,n} &= \phi_{j+1,n} - \phi_{j,n} \\ (\delta_x \phi)_{j,n} &= \phi_{j+1/2,n} - \phi_{j-1/2,n} \\ (\delta_t \phi)_{j,n+1/2} &= \phi_{j,n+1} - \phi_{j,n} \\ (\delta_t \phi)_{j,n} &= \phi_{j,n+1/2} - \phi_{j,n-1/2} \\ (\delta_t \delta_t \phi)_{j,n} &= (\delta_t \phi)_{j,n+1/2} - (\delta_t \phi)_{j,n-1/2} \\ &= \phi_{j,n+1} - 2\phi_{j,n} + \phi_{j,n-1} \end{aligned} \tag{39}$$

and so on. The difference formula for the equation of motion (33) is the following central difference formula:

$$\frac{\rho}{\Delta t^2}(\delta_t\delta_t w)_{j,n}=\frac{1}{\Delta x}(\delta_x\sigma)_{j,n}. \tag{40}$$

For (34),

$$\sigma_{j+1/2,n}=k\left(\alpha t+\frac{1}{\Delta x}(\delta_x w)_{j+1/2,n}\right)+2Y_{j+1/2,n}/3. \tag{41}$$

For (35),

$$\dot{e}_{j+1/2,n+1/2}=\frac{2}{3}\left(\alpha+\frac{1}{\Delta t\,\Delta x}(\delta_t\delta_x w)_{j+1/2,n+1/2}\right). \tag{42}$$

For (36),

$$\dot{e}_{j+1/2,n+1/2}=\dot{e}^{\mathrm{e}}_{j+1/2,n+1/2}+\dot{e}^{\mathrm{p}}_{j+1/2,n+1/2}. \tag{43}$$

For (37),

$$\dot{e}^{\mathrm{e}}_{j+1/2,n+1/2}=\frac{1}{3\mu\,\Delta t}(\delta_t Y)_{j+1/2,n+1/2}. \tag{44}$$

For (38), difference formulas of two general forms will be considered. The first is

$$Y_{j+1/2,n}=Y_0-\frac{2b\alpha}{3}+b\dot{e}^{\mathrm{p}}_{j+1/2,n-D}, \tag{45}$$

where D is either an integer or a half-integer. Since strain rates are centered at half-integer time steps, if D is an integer the above difference formula is defined to mean

$$Y_{j+1/2,n}=Y_0-\frac{2b\alpha}{3}+\frac{b}{2}(\dot{e}^{\mathrm{p}}_{j+1/2,n-D+1/2}+\dot{e}^{\mathrm{p}}_{j+1/2,n-D-1/2}). \tag{46}$$

If $D=\frac{3}{2}$, the difference formula (45) will be referred to as *backward-explicit*, since $Y_{j+1/2,n}$ depends only on quantities known from the two previous time steps.

If $D=\frac{1}{2}$, the difference formula will be called *backward-implicit*. It is implicit because in time step n, $\dot{e}^{\mathrm{p}}_{j+1/2,n-1/2}$ in (45), unlike $\dot{e}_{j+1/2,n-1/2}$, cannot be determined immediately from the known velocities $\dot{w}_{j,n-1/2}$. It is backward in the sense that the right side of (45) is located in time one half time step behind the left side.

If $D=0$, the difference formula (46) will be called *centered-implicit*, because it involves unknown velocities, and because the left and right sides of the equation are located at the same time steps.

By writing out the first few terms of the appropriate Taylor expansion, one finds that all the backward difference operators ($D>0$) discussed above for approximating $\dot{e}^{\mathrm{p}}$ have truncation error $O(\Delta t)$, while the central difference operator ($D=0$) has error $O(\Delta t^2)$. It will emerge that the $D=0$ method is unusable for reasons of numerical instability. This motivates a search for a stable differencing scheme for the plastic strain rate that retains the $O(\Delta t^2)$ properties of the $D=0$ method. A suitable approach is the following *three-point* method for evaluating the plastic strain rate:

$$Y_{j+1/2,n}=Y_0-\frac{2b\alpha}{3}+\frac{b}{2}(3\dot{e}^{\mathrm{p}}_{j+1/2,n-1/2}-\dot{e}^{\mathrm{p}}_{j+1/2,n-3/2}). \tag{47}$$

A Taylor expansion of this difference formula confirms that the truncation error is $O(\Delta t^2)$ as desired. It will be shown below that this method has no stability restriction beyond the CFL limit.

3. STABILITY AND ACCURACY ANALYSIS

In this section we simplify the system of difference equations (40)–(44) using the formulas (45), (46), and (47) to evaluate the rate-dependent yield stress. We consider first the formula for half-integer D, (45). We seek a single difference equation involving w only. After some lengthy algebraic manipulations, the details of which are given in [7], one arrives at the difference equation

$$\begin{aligned}&[(\delta_t\delta_t w)_{j,n}-C_b^2(\delta_x\delta_x w)_{j,n}]\\&\quad+R[(\delta_t\delta_t\delta_t w)_{j,n-D}-C_d^2(\delta_t\delta_x\delta_x w)_{j,n-D}]\\&\quad=0,\qquad D\in\mathscr{Z}_{1/2},\end{aligned} \tag{48}$$

where $\mathscr{Z}_{1/2}$ is the set of half-integers, and the Courant numbers corresponding to the bulk wave speed and dilatational wave speed are defined respectively by

$$\begin{aligned}C_b&=\sqrt{k\,\Delta t^2/\rho\,\Delta x^2},\\C_d&=\sqrt{(k+4\mu/3)\,\Delta t^2/\rho\,\Delta x^2}.\end{aligned} \tag{49}$$

The dimensionless constant R is defined by

$$R=\frac{b}{3\mu\,\Delta t}. \tag{50}$$

Equation (48) is a difference equation that involves only w and which is equivalent to the original system of difference equations for the model problem.

Repeating the simplification using the difference formula for integer D, (46), leads to the simplified difference equation

$$[(\delta_t\delta_t w)_{j,n} - C_b^2(\delta_x\delta_x w)_{j,n}] + \frac{R}{2}[(\delta_t\delta_t\delta_t w)_{j,n-D+1/2} - C_d^2(\delta_t\delta_x\delta_x w)_{j,n-D+1/2}] + \frac{R}{2}[(\delta_t\delta_t\delta_t w)_{j,n-D-1/2} - C_d^2(\delta_t\delta_x\delta_x w)_{j,n-D-1/2}] = 0, \quad D \in \mathscr{Z}, \tag{51}$$

where $\mathscr{Z}$ is the set of integers.

Repeating the process for the three-point method (47) results in the following simplified difference equation for w:

$$[(\delta_t\delta_t w)_{j,n} - C_b^2(\delta_x\delta_x w)_{j,n}] + \frac{3R}{2}[(\delta_t\delta_t\delta_t w)_{j,n-1/2} - C_d^2(\delta_t\delta_x\delta_x w)_{j,n-1/2}] - \frac{R}{2}[(\delta_t\delta_t\delta_t w)_{j,n-3/2} - C_d^2(\delta_t\delta_x\delta_x w)_{j,n-3/2}] = 0. \tag{52}$$

A few observations about these simplified difference equations are of interest:

1. The case $R = 0$, i.e., $b = 0$, corresponds to constant Y. In this case the difference equations reduce to the appropriate equation for the wave equation with the wave velocity equal to the bulk wave speed.

2. The case $R \to \infty$, i.e., $b \to \infty$, corresponds to an elastic material. This is because according to (45) or its analogues an infinitely large value of b forces $\dot{e}^p$ to be zero; hence all the strain is elastic. In this case the difference equations reduce to the appropriate difference equation for the wave equation with the wave velocity equal to the dilatational wave speed.

3. $C_b \leqslant C_d$ because of (49), and because $\mu \geqslant 0$ for all reasonable materials.

4. The case $C_b = C_d$ would correspond physically to a metal near its melting point, at which $\mu \approx 0$. It would also correspond to rubbery materials.

5. If in the difference equations we set $C_b = 0$ and replace C_d by the Courant number for shear waves, $C_s = \sqrt{\mu\,\Delta t^2/\rho\,\Delta x^2}$, then the result gives the difference equations for shear waves. This may be shown by setting $k = 0$ in (34).

6. The stability of the difference equations can only depend on C_b, C_d, and R; R is the only one of these constants that involves the viscoplastic parameter b. Note from (50) that R involves Δt but not Δx. Since as a minimum we need a method that is stable when b and Δt are arbitrarily small, a useful numerical method cannot have any stability restriction on R. Some restriction on C_d or C_b, in addition to the usual condition $C_d \leqslant 1$, might be acceptable.

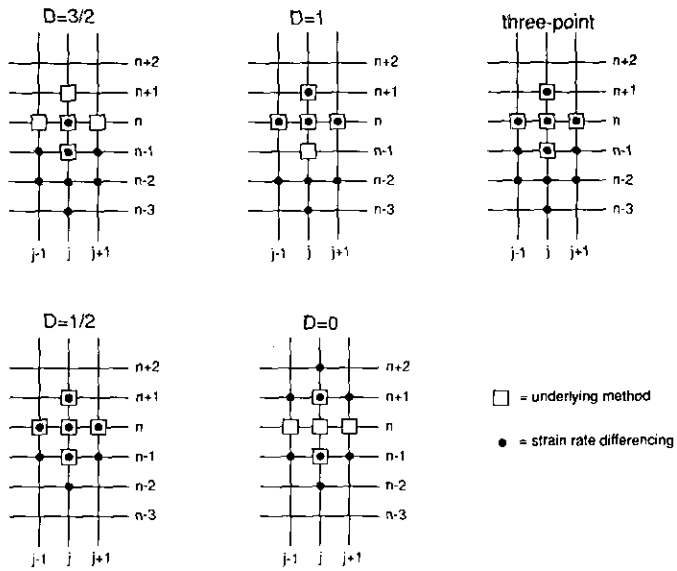

FIG. 1. Finite difference molecules for the difference equations. The "underlying method" refers to explicit central differencing of the wave equation.

Finite difference molecules for the difference equations are shown in Fig. 1.

We now turn to an analysis of the accuracy of the methods. By elementary manipulations similar to those used to simplify the difference relations above, the system of partial differential equations (33)–(38) may be simplified to

$$(\ddot{w} - c_b^2 w_{xx}) + r(\ddot{w} - c_d^2 \ddot{w}_{xx}) = 0, \tag{53}$$

where

$$r = \frac{b}{3\mu}, \qquad c_b = \sqrt{k/\rho}, \qquad c_d = \sqrt{(k + 4\mu/3)/\rho}. \tag{54}$$

By writing out a few terms of the Taylor expansions for various difference operators, one finds

$$\frac{(\delta_t\delta_t w)_{j,n}}{\Delta t^2} = \ddot{w}(x_j, t_n) + O(\Delta t^2)$$

$$\frac{(\delta_x\delta_x w)_{j,n}}{\Delta x^2} = w_{xx}(x_j, t_n) + O(\Delta x^2)$$

$$\frac{(\delta_t\delta_t\delta_t w)_{j,n-D}}{\Delta t^3} = \ddot{w}(x_j, t_n) + O(\Delta t) \qquad \text{for} \quad D > 0$$

$$\frac{(\delta_t\delta_t\delta_t w)_{j,n}}{\Delta t^3} = \ddot{w}(x_j, t_n) + O(\Delta t^2)$$

$$\frac{3}{2}\frac{(\delta_t\delta_t\delta_t w)_{j,n-1/2}}{\Delta t^3}-\frac{1}{2}\frac{(\delta_t\delta_t\delta_t w)_{j,n-3/2}}{\Delta t^3}$$
$$=\ddot{w}(x_j,t_n)+O(\Delta t^2)$$
$$\frac{(\delta_t\delta_x\delta_x w)_{j,n-D}}{\Delta t\,\Delta x^2}$$
$$=\dot{w}_{xx}(x_j,t_n)+O(\Delta t)+O(\Delta x^2)\qquad \text{for}\quad D>0$$
$$\frac{(\delta_t\delta_x\delta_x w)_{j,n}}{\Delta t\,\Delta x^2}$$
$$=\dot{w}_{xx}(x_j,t_n)+O(\Delta t^2)+O(\Delta x^2)$$
$$\frac{3}{2}\frac{(\delta_t\delta_x\delta_x x)_{j,n-1/2}}{\Delta t\,\Delta x^2}-\frac{1}{2}\frac{(\delta_t\delta_x\delta_x w)_{j,n-3/2}}{\Delta t\,\Delta x^2}$$
$$=\dot{w}_{xx}(x_j,t_n)+O(\Delta t^2)+O(\Delta x^2). \tag{55}$$

Now observe that the difference equation for half-integer D, (48), may be written as

$$\left[\frac{(\delta_t\delta_t w)_{j,n}}{\Delta t^2}-c_b^2\frac{(\delta_x\delta_x w)_{j,n}}{\Delta x^2}\right]$$
$$+r\left[\frac{(\delta_t\delta_t\delta_t w)_{j,n-D}}{\Delta t^3}-c_d^2\frac{(\delta_t\delta_x\delta_x w)_{j,n-D}}{\Delta t\,\Delta x^2}\right]=0. \tag{56}$$

Substituting the appropriate operators with half-integer D from (55) into (56) and rearranging yields

$$(\ddot{w}-c_b^2 w_{xx})+r(\ddot{w}-c_d^2\dot{w}_{xx})=O(\Delta t)+O(\Delta x^2). \tag{57}$$

Therefore all the methods with half-integer D have error $O(\Delta t)+O(\Delta x^2)$.

Proceeding similarly for the methods with integer $D>0$, one finds that the error is also $O(\Delta t)+O(\Delta x^2)$. However, for $D=0$, and for the three-point method, the error is $O(\Delta t^2)+O(\Delta x^2)$. The above results are summarized in Table I.

We now investigate the numerical stability of the difference formulas (48), (51), and (52). Following the usual procedure for a von Neumann stability analysis [8], we assume that for any j and n,

$$w_{j,n}=\zeta^n e^{ij\gamma}, \tag{58}$$

where ζ is a possibly complex constant called the *amplification factor*, γ is a positive constant, $i=\sqrt{-1}$, and the superscripts indicate powers. We require $|\zeta|\leqslant 1$ for numerical stability for all values of γ.

The remainder of the analysis is concerned with evaluating ζ from the difference formulas. We start with (48). Substituting (58) into (48) and using the identity $\cos\theta=(\exp(i\theta)+\exp(-i\theta))/2$, we find that for half-integer D,

$$[(\zeta-1)^2-2C_b^2(\cos\gamma-1)\zeta]+R\zeta^{-D-1/2}(\zeta-1)$$
$$\times[(\zeta-1)^2-2C_d^2(\cos\gamma-1)\zeta]=0. \tag{59}$$

Similarly, for integer D, (51) yields

$$[(\zeta-1)^2-2C_b^2(\cos\gamma-1)\zeta]$$
$$+\frac{R}{2}\zeta^{-D-1}(\zeta+1)(\zeta-1)$$
$$\times[(\zeta-1)^2-2C_d^2(\cos\gamma-1)\zeta]=0. \tag{60}$$

For the three-point method, (52) leads to

$$[(\zeta-1)^2-2C_b^2(\cos\gamma-1)\zeta]$$
$$+\frac{R}{2}\zeta^{-2}(3\zeta-1)(\zeta-1)$$
$$\times[(\zeta-1)^2-2C_d^2(\cos\gamma-1)\zeta]=0. \tag{61}$$

For the methods of interest, (59), (60), and (61) yield a polynomial in ζ of degree L with $L=3$ or $L=4$. Denote the roots of the polynomial by

$$\zeta_1(C_d,C_b,\gamma,R),\ldots,\zeta_L(C_d,C_b,\gamma,R). \tag{62}$$

Let a function Z be defined by

$$Z(C_d,C_b)=\max_{0\leqslant\gamma\leqslant\pi,\,R\geqslant 0,\,1\leqslant l\leqslant L}(|\zeta_l(C_d,C_b,\gamma,R)|). \tag{63}$$

Recall that for numerical stability we require $|\zeta|\leqslant 1$ for all choices of the constants γ and R in these equations. Therefore the method is stable in this sense for a given pair of Courant numbers C_d, C_b if $Z(C_d,C_b)\leqslant 1$ and unstable otherwise.

It is easy to evaluate $Z(C_d,C_b)$ approximately by sampling large numbers of choices of γ and R and using standard formulas for the exact roots of cubic and quartic

TABLE I

Truncation Error and Region of Stability ($Z\leqslant 1$) for Some Differencing Schemes

Method	Error	Region of stability
$D=0$ (centered-implicit)	$O(\Delta t^2,\Delta x^2)$	$\varnothing$
$D=1/2$ (backward-implicit)	$O(\Delta t,\Delta x^2)$	$0\leqslant C_d\leqslant 1, 0\leqslant C_b\leqslant C_d$
$D=1$	$O(\Delta t,\Delta x^2)$	$0\leqslant C_d\leqslant 1/\sqrt{2}, 0\leqslant C_b\leqslant C_d$
$D=3/2$ (backward-explicit)	$O(\Delta t,\Delta x^2)$	$\varnothing$
Three-point	$O(\Delta t^2,\Delta x^2)$	$0\leqslant C_d\leqslant 1, 0\leqslant C_b\leqslant C_d^2$

polynomials. By carrying out this procedure for many choices of C_d and C_b, it is also straightforward to demonstrate what choices of these variables, if any, assure numerical stability.

This procedure was carried out for the three-point method and for the following choices of D: $\frac{3}{2}$, 1, $\frac{1}{2}$, and 0. The results are summarized in Table I. The notation $\varnothing$ for the region of stability indicates unconditional instability.

Note that the condition $0 \leqslant C_b \leqslant C_d$ is automatically satisfied for all real materials because $\mu \geqslant 0$ (see (49)). Also note that the stability conditions for the $D = \frac{1}{2}$ (backward-implicit) and three-point methods are simply the usual CFL condition.

A small Lagrangian wavecode was written to demonstrate the backward-implicit and three-point methods for the model problem described above. There were 100 nodes. The boundary condition was a step function for $\dot{w}$ on the left boundary. The parameters were as follows:

$$\begin{aligned} C_d &= 0.9 \\ C_b &= 0.7868 \\ k &= 1 \\ \mu &= 0.4615 \\ Y_0 &= 1 \\ \rho &= 1 \\ \alpha &= 1 \\ b &= 0.3. \end{aligned} \tag{64}$$

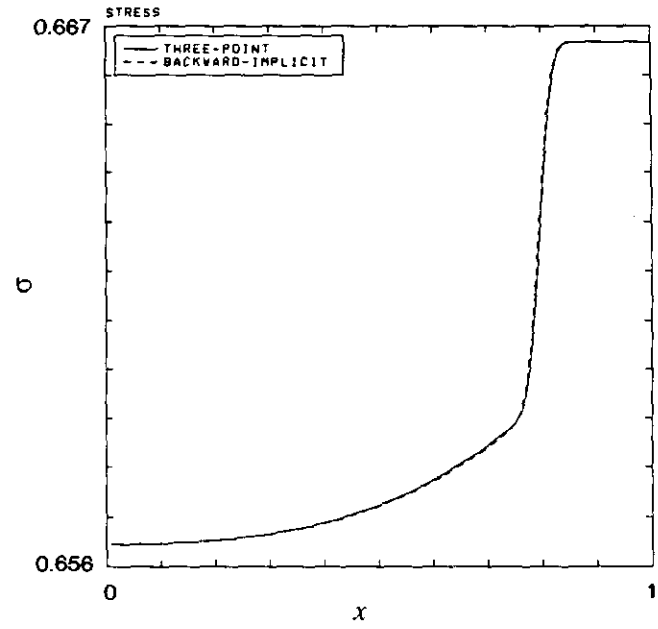

FIG. 3. Stress as a function of distance in the example problem.

Figure 2 shows the velocity $\dot{w}$ as a function of x after the wave has propagated most of the distance through the mesh. The solid line is for the three-point method, and the dashed line is for the backward-implicit method. The rate-dependence of the constitutive model clearly causes rapid decay of the shock wave. Figure 3 shows the stress σ as a function of x, and Fig. 4 shows the plastic strain rate.

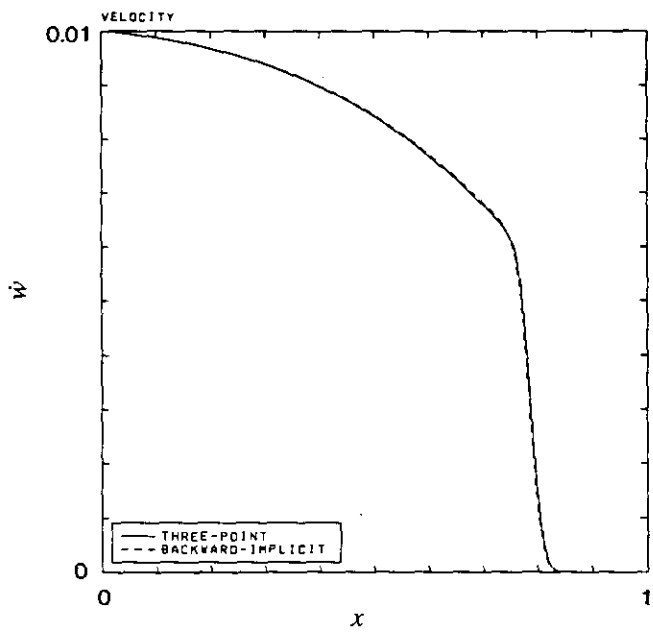

FIG. 2. Velocity as a function of distance in the example problem.

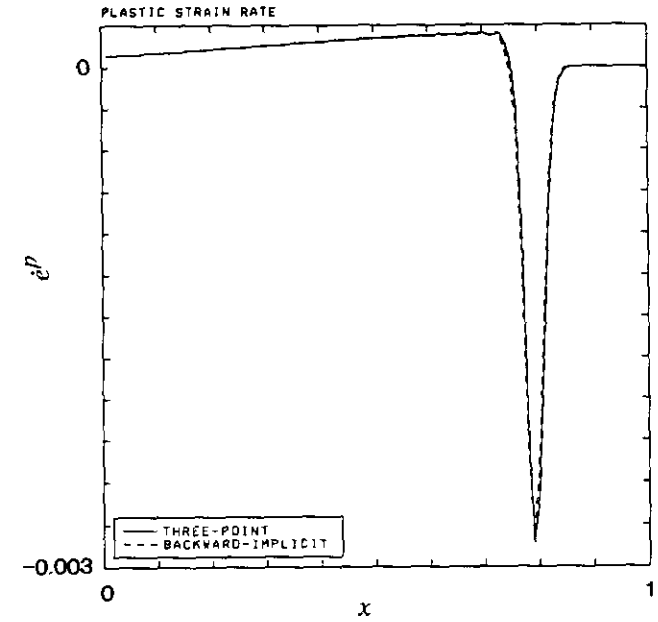

FIG. 4. Plastic strain rate as a function of distance in the example problem.

4. GENERALIZATION TO MULTIPLE DIMENSIONS

Of the methods investigated, only the backward-implicit and the three-point methods had no restriction on the time step size beyond the usual CFL condition. Of these, the three-point method had better truncation error. However, the three-point method requires additional data to be stored, since in practice the plastic strain rate term is evaluated from

$$\begin{aligned}\dot{e}^{\mathrm{p}}_{j,n} &= \frac{3}{2}\dot{e}^{\mathrm{p}}_{j,n-1/2} - \frac{1}{2}\dot{e}^{\mathrm{p}}_{j,n-3/2} \\ &= \frac{3}{2}\frac{e^{\mathrm{p}}_{j,n} - e^{\mathrm{p}}_{j,n-1}}{\Delta t} - \frac{1}{2}\frac{e^{\mathrm{p}}_{j,n-1} - e^{\mathrm{p}}_{j,n-2}}{\Delta t} \\ &= \frac{1}{2\Delta t}(3e^{\mathrm{p}}_{j,n} - 4e^{\mathrm{p}}_{j,n-1} + e^{\mathrm{p}}_{j,n-2}). \end{aligned} \tag{65}$$

Therefore the plastic strains from *two* previous time steps must be retained, while the backward-implicit method requires the data from only *one* previous time step.

In large three-dimensional calculations, even with modern computers, the need for memory for an additional array dimensioned to the size of the mesh can represent a significant burden, and one would like to avoid adding such an array if possible. In order to gain some insight into the trade-off between improved accuracy and the need for an extra array, a series of test problems was run with both methods. The problems included both coarse and fine meshes and focused mainly on shock wave propagation. These tests showed virtually no difference in the results with the two methods. Therefore the backward-implicit method appears to be adequate for general-purpose multi-dimensional wavecodes, and this method was the one implemented in CTH.

As Table I shows, the $D = 1$ method is stable over a useful region, but its stability condition is more restrictive than that of the backward-implicit and three-point methods. The $D = 1$ method appears to have no advantages, and it was not pursued further. The remainder of this section concerns the implementation of the backward-implicit differencing scheme in CTH.

The generalization of (45) with $D = \frac{1}{2}$ to multiple dimensions and to nonlinear constitutive relations is found from (10) with the appropriate difference formula for plastic strain rate,

$$Y_{i,j,k,n} = Y\left(T_{i,j,k,n-1}, \varepsilon^{\mathrm{p}}_{i,j,k,n-1}, \frac{\varepsilon^{\mathrm{p}}_{i,j,k,n} - \varepsilon^{\mathrm{p}}_{i,j,k,n-1}}{\Delta t_{n-1/2}}\right), \tag{66}$$

where i, j, k identify an Eulerian three-dimensional cell. The quantity $T_{i,j,k,n-1}$ appears instead of $T_{i,j,k,n}$ in (66) because the architecture of CTH is such that $T_{i,j,k,n}$ is not known at the point in the computational sequence where $Y_{i,j,k,n}$ is evaluated. The second argument of Y is also evaluated at time step $n-1$ because in practice strain hardening causes such a slowly varying dependence of Y on ε^{p} that a more accurate evaluation of this term would not result in a significant improvement in accuracy, although it would considerably complicate the calculations.

In the remainder of this discussion, the cell indices will be omitted, since there is only one cell involved. Also, we will use the following less cumbersome notation: $\Delta\phi_n = (\delta_t\phi)_n$, $\Delta\phi_{n+1/2} = (\delta_t\phi)_{n+1/2}$.

Since $\varepsilon^{\mathrm{p}}_n$ depends on Y_n, the difference formula in (66) gives Y_n only implicitly.

Let $\Delta\mathbf{e}_{n-1/2}$ be the total deviatoric strain increment tensor for a cell. Let $\mathbf{S}_{n-1}$ be the old deviatoric stress tensor. Both $\Delta\mathbf{e}_{n-1/2}$ and $\mathbf{S}_{n-1}$ are known at the point in the computational sequence at which Y_n is to be evaluated.

In order to avoid elaborate tensor computations, we would like to recast the problem in such a way that only scalars are involved. To do this, we proceed as follows. First, we write the flow rule for yielded material (9) as

$$\dot{\mathbf{e}}^{\mathrm{p}} = \dot{e}^{\mathrm{p}}\frac{\mathbf{S}}{S}, \tag{67}$$

where $\dot{e}^{\mathrm{p}} = |\dot{\mathbf{e}}^{\mathrm{p}}|$ and

$$S = |\mathbf{S}| = \sqrt{S_{ij}S_{ij}}. \tag{68}$$

Now define a scalar $\dot{e}$ by

$$\dot{e} = \frac{\dot{\mathbf{e}}\cdot\mathbf{S}}{S}. \tag{69}$$

Combining this with (67) the decomposition (5) results in

$$\dot{e} = \dot{e}^{\mathrm{e}} + \dot{e}^{\mathrm{p}}, \tag{70}$$

where

$$\dot{e}^{\mathrm{e}} = \frac{\dot{\mathbf{e}}^{\mathrm{e}}\cdot\mathbf{S}}{S}. \tag{71}$$

Differentiating (68) with respect to time gives

$$\dot{S} = \frac{\dot{\mathbf{S}}\cdot\mathbf{S}}{S}. \tag{72}$$

A generalization of (7) to large deformation gradients is

$$\dot{\mathbf{e}}^{\mathrm{e}} = \frac{1}{2\mu}(\dot{\mathbf{S}} + \mathbf{SW} - \mathbf{WS}), \tag{73}$$

where $\mathbf{W}$ is the spin tensor, defined by

$$\mathbf{W} = \tfrac{1}{2}(\nabla \mathbf{v} - (\nabla \mathbf{v})^{\mathrm{T}}), \tag{74}$$

where $\mathbf{v}$ is the Eulerian velocity vector field. The term in parentheses in (73) is the Jaumann stress rate. The terms involving spin arise because rigid rotations at a point in a body cause a change in the stress tensor even though they do not affect the strain rate. See Ref. [9] for a discussion of the Jaumann stress rate. Substituting (73) into (71) and making use of (72) yields

$$\dot{S} = 2\mu \dot{e}^{\mathrm{e}}. \tag{75}$$

Note that the spin terms have dropped out of (75). This is because the following identity holds for any symmetric tensor $\mathbf{S}$ and any tensor $\mathbf{W}$:

$$(\mathbf{SW} - \mathbf{WS}) \cdot \mathbf{S} = 0. \tag{76}$$

The proof of this is easily performed using index notation. Geometrically, (76) simply means that the spin terms in the stress rate are parallel to the yield surface.

In the numerical method it is more convenient to use strain increments than strain rates. Define the total deviatoric strain increment by

$$\Delta \mathbf{e}_{n-1/2} = \dot{\mathbf{e}}_{n-1/2}\, \Delta t, \tag{77}$$

with other incremental quantities derived similarly in terms of rates. Equation (69) is replaced by

$$\Delta e_{n-1/2} = \frac{\Delta \mathbf{e}_{n-1/2} \cdot \mathbf{S}_{n-1}}{S_{n-1}}. \tag{78}$$

Note that $\Delta e_{n-1/2}$ can be evaluated immediately in time step n. Equation (70) is replaced by

$$\Delta e_{n-1/2} = \Delta e^{\mathrm{e}}_{n-1/2} + \Delta e^{\mathrm{p}}_{n-1/2}. \tag{79}$$

Equation (75) is replaced by

$$\Delta e^{\mathrm{e}}_{n-1/2} = \frac{S_n - S_{n-1}}{2\mu}. \tag{80}$$

If at the end of time step n the material is yielded, it follows from (8) and (80) that

$$\Delta e^{\mathrm{e}}_{n-1/2} = \frac{\sqrt{2/3}\, Y_n - S_{n-1}}{2\mu}. \tag{81}$$

The increment of equivalent plastic strain is found from (11) and (67) to be

$$\Delta \varepsilon^{\mathrm{p}}_{n-1/2} = \sqrt{\tfrac{2}{3}}\, \Delta e^{\mathrm{p}}_{n-1/2}. \tag{82}$$

The yield stress is computed from (66) and (82) as

$$Y_n = Y\left(T_{n-1}, \varepsilon^{\mathrm{p}}_{n-1}, \sqrt{\frac{2}{3}} \frac{\Delta e^{\mathrm{p}}_{n-1/2}}{\Delta t_{n-1/2}}\right). \tag{83}$$

The three equations (79), (81), and (83) form a nonlinear algebraic system in which the unknowns are $\Delta e^{\mathrm{e}}_{n-1/2}$, $\Delta e^{\mathrm{p}}_{n-1/2}$, and Y_n. The solution of this system is readily found by Newton's method.

In practice, there are certain cases in which the method described in this section fails to give a meaningful value of Y_n. These cases most frequently arise under the following conditions:

- An Eulerian cell is not filled with a single material. In this case the values of node velocity, which are used in finding the strain rates, are unreliable because they may refer to void or to a different material.
- Numerical noise causes the arguments of the function Y to be out of the range of validity of the constitutive model.

When either of these conditions is detected, some special procedure must be used to find a reasonable value for Y_n. Often it is possible to omit the rate-dependent terms in Y, retaining the dependence on equivalent plastic strain and temperature. In metals, Y is a slowly varying function of these quantities, so the omission of the rate-dependent terms is a reliable way to obtain meaningful values of yield stress when either of the two conditions listed above holds.

Once Y_n is known, the deviatoric stress tensor in a cell is evaluated according to the method introduced by Wilkins [10]. The method is applied as though the yield stress were a constant. This method is summarized here for completeness.

First, an "elastic estimate" $\mathbf{S}^{\mathrm{e}}_n$ of the new deviatoric stress tensor is obtained based on the assumption that the material is elastic during the incremental deformation that occurred during the time step. Differencing (73), we obtain

$$\mathbf{S}^{\mathrm{e}}_n = \mathbf{S}_{n-1} + 2\mu\, \Delta \mathbf{e}^{\mathrm{e}}_{n-1/2} + \Delta t_{n-1/2} \times (\mathbf{W}_{n-1/2}\mathbf{S}^{\mathrm{e}}_{n-1/2} - \mathbf{S}^{\mathrm{e}}_{n-1/2}\mathbf{W}_{n-1/2}), \tag{84}$$

where

$$\mathbf{S}^{\mathrm{e}}_{n-1/2} = \tfrac{1}{2}(\mathbf{S}_{n-1} + \mathbf{S}^{\mathrm{e}}_n) \tag{85}$$

and $\mathbf{W}$ is the spin tensor, defined in (74). In multi-dimensional calculations, finding $\mathbf{S}_n^e$ requires solving a non-homogeneous linear algebraic system of equations derived from (84) and (85).

The next step is to find $\mathbf{S}_n$, the new deviatoric stress tensor. The cases of non-yielded and yielded $\mathbf{S}_n^e$ are treated as follows:

$$\mathbf{S}_n = \begin{cases} \mathbf{S}_n^e, & |\mathbf{S}_n^e| < \sqrt{2/3}\, Y_n \\ \sqrt{2/3}\, Y_n \mathbf{S}_n^e / |\mathbf{S}_n^e|, & |\mathbf{S}_n^e| \geqslant \sqrt{2/3}\, Y_n. \end{cases} \tag{86}$$

Geometrically, the second of (86) represents "putting the stress state back on the yield surface." This method of computing the deviatoric stress ensures that any stress state lies within or on the yield surface, and it correctly accounts for the elastic straining and rigid rotation.

The only computation left to perform in time step n is to find the new value of ε^p. We can do this without involving the spin terms. By taking the tensor dot product of both sides of (67) with $\mathbf{S}/S$ and by using (73), (5), and (76),

$$\begin{aligned} \dot{e}^p &= \mathbf{e}^p \cdot \frac{\mathbf{S}}{S} \\ &= (\dot{\mathbf{e}} - \dot{\mathbf{e}}^e) \cdot \frac{\mathbf{S}}{S} \\ &= \left[\dot{\mathbf{e}} - \frac{1}{2\mu} (\dot{\mathbf{S}} + \mathbf{SW} - \mathbf{WS}) \right] \cdot \frac{\mathbf{S}}{S} \\ &= \left[\dot{\mathbf{e}} \cdot \mathbf{S} - \frac{1}{2\mu} (\dot{\mathbf{S}} + \mathbf{SW} - \mathbf{WS}) \cdot \mathbf{S} \right] \frac{1}{S} \\ &= \left[\dot{\mathbf{e}} \cdot \mathbf{S} - \frac{\dot{\mathbf{S}}}{2\mu} \cdot \mathbf{S} \right] \frac{1}{S} \\ &= \left[\dot{\mathbf{e}} - \frac{\dot{\mathbf{S}}}{2\mu} \right] \cdot \frac{\mathbf{S}}{S}. \end{aligned} \tag{87}$$

The differenced form of this is

$$\Delta e^p_{n-1/2} = \left[\Delta \mathbf{e}_{n-1/2} - \frac{\Delta \mathbf{S}_{n-1/2}}{2\mu} \right] \cdot \frac{\mathbf{S}_{n-1/2}}{S_{n-1/2}}, \tag{88}$$

where

$$\Delta \mathbf{S}_{n-1/2} = \mathbf{S}_n - \mathbf{S}_{n-1} \tag{89}$$

$$\mathbf{S}_{n-1/2} = \frac{\mathbf{S}_n + \mathbf{S}_{n-1}}{2}. \tag{90}$$

At this point in the calculation, $\mathbf{S}_n$ is known, so the indicated quantities can be computed immediately. Finally, the new value of equivalent plastic strain is found from the above and from numerical integration of (11):

$$\varepsilon_n^p = \varepsilon_{n-1}^p + \sqrt{\tfrac{2}{3}}\, \Delta e^p_{n-1/2}. \tag{91}$$

Although it would be possible in many cases to use the value of $\Delta \varepsilon^p_{n-1/2}$ from (82) to integrate equivalent plastic strain, the method described here is more general because of the special cases in which a rate-dependent calculation is impossible, as discussed above. In these special cases (82) does not give meaningful values of $\Delta \varepsilon^p_{n-1/2}$, but it is usually still possible to find a useful approximate value of Y_n. Therefore (91) remains useful in these special cases.

5. CONCLUSIONS

The results described in this paper provide an analysis of the stability and accuracy of a family of differencing methods for the rate-dependent term in viscoplastic constitutive laws. As shown in Table I, the different methods within this family vary in their accuracy and ranges of stability.

Two differencing schemes usable in wavecodes have been identified and tested. These methods are the backward-implicit scheme, which is first-order accurate, and the three-point scheme, which is second-order accurate. The latter requires more storage than the former and, in practice, its improved accuracy does not appear to be required for a general-purpose wavecode.

The backward-implicit scheme has been implemented in CTH, a three-dimensional Eulerian wavecode. For each cell, an iteration is required to evaluate the current yield stress in each cycle. In typical CTH calculations using the Johnson–Cook or Zerilli–Armstrong models, this iteration adds about 4% to the computer time. However, because no interaction between cells occurs in the formulation of the constitutive law, there is no need to solve a large set of linear equations in each time step as would be necessary in an implicit code. In this sense the backward-implicit or three-point schemes can be integrated easily into a typical wavecode.

For use in wavecodes, the ideal differencing scheme for the rate-dependent term would be fully explicit, i.e., it would allow the yield stress to be computed immediately from known data without any iteration. No such fully explicit scheme that is numerically stable has been identified in this study. However, since the family of methods considered here is not exhaustive, it is possible that such a method exists.

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