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On the Numerical Implementation of CONF-801207--2
 Inelastic Time Dependent and Time Independent, CONF-801159--1
 Finite Strain Constitutive Equations in Solids*

MASTER

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Abstract

A number of complex issues are addressed which will allow the incorporation of finite strain, inelastic material behavior into the piecewise numerical construction of solutions in solid mechanics. Without recourse to extensive continuum mechanics preliminaries, an elementary time independent plasticity model, an elementary time dependent creep model, and a viscoelastic model are introduced as examples of constitutive equations which are routinely used in engineering calculations. The constitutive equations are all suitable for problems involving large deformations and finite strains. The plasticity and creep models are in rate form and use the symmetric part of the velocity gradient or the stretching to compute the co-rotational time derivative of the Cauchy stress. The viscoelastic model computes the current value of the Cauchy stress from a hereditary integral of a "materially invariant" form of the stretching history. The current configuration is selected for evaluation of equilibrium as opposed to either the reference configuration or the last established equilibrium configuration. The process of strain incrementation is examined in some depth and the stretching evaluated at the midinterval multiplied by the time step is identified as the appropriate finite strain increment to use with the selected form of the constitutive equations. Discussed is the conversion of rotation rates based on the spin into incremental orthogonal rotations which are then used to update stresses and state variables due to rigid body rotation during the load increment. Comments and references to the literature are directed at numerical integration of the constitutive equations with an emphasis on doing this accurately, if not exactly, for any time step and stretching. This material taken collectively provides an approach to numerical implementation which is marked by its simplicity.

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1. INTRODUCTION

Successful engineering calculations which incorporate inelastic material behavior require that a number of complex issues be addressed. The first is a mathematical statement of observed and measured material behavior known as a constitutive model. Constitutive modeling has a history and a formalism which is separate from and predates recent work on numerical implementation. There is a wealth of literature on constitutive models and extensive writings in continuum mechanics guiding the formulation of the equations which mimic observed material behavior. It is assumed the reader has some familiarity with this literature.

Three very elementary constitutive models will be used here for the purposes of example and little reference to the depth of the literature in each of the respective areas will be made. In particular, a representative time independent plasticity model, a viscoelastic model, and a time dependent creep model will be cited.

After a review of the mechanics which will be needed the focus will be on the issues related to numerical implementation. The goal is to develop a predictive capability. Specifically, the incremental integration of these equations which accompanies the piecewise "construction" of solutions in static, quasistatic and dynamic boundary value problems will be addressed. The incrementation in strain, the interface needed between the numerical implementation of the constitutive equations and the balance of the boundary value problem, and the numerical procedures used for integrating the respective constitutive models are discussed in turn. It is the numerical implementation which allows the plethora of constitutive proposals to be used in practice. The limitations of space will only permit an exposition of one sequence of possible choices from among the many possible.

Notation. The treatment of continuum mechanics used here follows closely that found in Truesdell & Toupin [1]. A body V is given which occupies a finite region of Euclidian space. Subjected to prescribed body forces and surface tractions, the body V undergoes the motion $x^i = \chi^i(X^\alpha, t)$. The particles of the body are identified by the coordinates X^α . They are referred to as material coordinates, and the relation of the particles to the coordinates X^α does not change in time. The places in space which the particles occupy during the motion are identified by the coordinates x^i . The function χ^i describes the motion of the particles X^α through space as a function of time t . It is the motion χ^i which is sought. The place occupied by the body at $t = 0$ is taken as the reference configuration. In this configuration the body is assumed to be strain free, though not necessarily stress free. Only material coordinates X^α which coincide with the spatial coordinates x^i in the reference configuration are considered. Thus, in the reference configuration, $\chi^i(X^\alpha, 0) \equiv X^\alpha$.

The covariant and contravariant components of the metric tensor for the spatial coordinates x^i are g_{rs} and g^{rs} , respectively, while in the coordinates of the reference configuration they are $G_{\alpha\beta}$ and $G^{\alpha\beta}$, respectively. In what follows, the spatial coordinates and the current configuration of the body will be used for strain rate, stress, stress rate and equilibrium.

Strain and Strain Rate. In finite deformations there are many strain measures which are useful. The majority of them can be computed from the deformation gradient F^k defined by

$$F^k = \frac{\partial x^k}{\partial X^\alpha} (X^\beta, t) . \quad (1)$$

The velocity v^k is defined as

$$v^k(X^\alpha, t) \equiv \frac{\partial x^k}{\partial t} (X^\alpha, t) . \quad (2)$$

The stretching is given by

$$d_{km} = \frac{1}{2} (v_{k,m} + v_{m,k}) , \quad (3)$$

with the spin given by

$$w_{km} = \frac{1}{2} (v_{k,m} - v_{m,k}) . \quad (4)$$

The comma in $v_{k,m}$ denotes covariant differentiation. In the constitutive models which follow, the stretching is used as a strain rate measure. There are a wealth of additional strain and strain rate variables which could be introduced but they are not needed here.—Further references to them can be found in Truesdell and Toupin [1].

2. CONSTITUTIVE THEORIES

The stress relations considered are those of elementary character. They represent three classical forms of material behavior and are remarkably adaptable in performing useful engineering analyses. They are classical plasticity which exhibits path dependent but time independent behavior, classical viscoelasticity, and classical creep both of which have path dependent and time dependent behavior. These attributes have important consequences when incremental strategies are considered.

Plasticity. Plasticity is the behavior characteristic of ductile metals. Figure 1 shows results which are typical of the behavior of a metal bar loaded first in uniaxial tension followed by uniaxial compression. The straight line representation in Figure 1 is an idealization of this behavior. This is the approximation which results from the plasticity relations employed here, Goel and Malvern [2]. It is based on the notion of a universal hardening curve from which general triaxial behavior is predicted. The finite strain treatment of Key, Krieg, and Biffle [3] is used. It is stated in a rate form where the invariant co-rotational or Jaumann stress rate is related through a tangent modulus to the stretching. The result is equation (5).

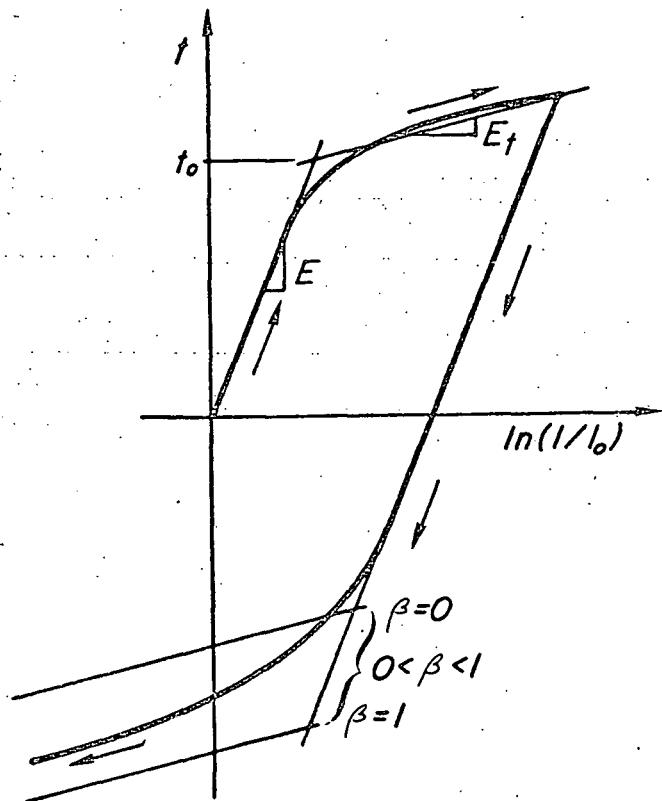


Figure 1. The typical behavior of a ductile metal bar loaded first in uniaxial tension followed by uniaxial compression. The straight line approximation is characterized as an elastic modulus E , a yield stress t_0 , a strain hardening modulus E_t , and a hardening parameter β where kinematic hardening is obtained with $\beta = 0$, isotropic hardening is obtained with $\beta = 1$, and a linear combination of the two is obtained for β between zero and one.

$$\nabla t^{rs} = t^{rs} - w_m^r t^{ms} + t^{rm} w_m^s = C^{rsmn} d_{mn} \quad (5)$$

When no yielding is occurring, C^{rsmn} is the isotropic tensor $\lambda g^{rs} g^{mn} + 2\mu g^{rm} g^{sn}$, where λ and μ are the Lame' parameters. When plastic flow is occurring, that is, when $\frac{1}{2} \xi'_{ij} \xi'^{-1} ij - k^2 = 0$ and $\xi'_{rs} \nabla \xi'^{rs} > 0$, the tangent modulus is given by

$$C^{rsmn} = \lambda g^{rs} g^{mn} + 2\mu (g^{rm} g^{sn} - n^{rs} n^{mn}) \quad (6)$$

where

$$n^{rs} = \xi^{rs}/[2k^2(1 + H/3\mu)]^{1/2} ,$$

$$\xi'_{rs} = t'_{rs} - \alpha'_{rs} ,$$

$$\sqrt{2k} = \beta \frac{2}{3} H |d_{rs}^p| , \quad k(0) = (2/3)^{1/2} t_0 ,$$

$$\nabla \alpha_{rs} = (1 - \beta) \frac{2}{3} H d_{rs}^p , \quad \alpha_{rs}(0) = 0 .$$

Isotropic hardening is described by $\beta = 1$. Kinematic hardening is included in a rather obvious way by letting $\beta = 0$ and prescribing the center of the yield surface α_{ij} to move according to $\nabla \alpha_{ij} = (1 - \beta) \frac{2}{3} H d_{rs}^p$. The prime denotes deviatoric components, the superscript p denotes the plastic part of the stretching, and $H = E E_t / (E - E_t)$.

Viscoelasticity. Viscoelasticity is the behavior characteristic of polymeric materials. Under a constant stress they creep and under a constant strain, the stress relaxes. The bulk behavior is much less viscoelastic than the deviatoric response and is therefore often taken to be elastic. Thus,

$$t_i^1 = 3k \ln \left(\frac{\rho_0}{\rho} \right) , \quad (7)$$

where k is the bulk modulus, ρ is the density in the current configuration, and ρ_0 is the density in the reference configuration.

Since the material, in general, is rotating relative to the spatial coordinates, the stretching history does not describe a material fiber history suitable for use in a hereditary integral. A rotationally invariant form of the stretching must be introduced. A suitable rotation comes from the polar decomposition of the deformation gradient. Thus,

$$F_\alpha^h = R^{hm} V_{ma} \quad (8)$$

where R^{hm} is an orthogonal rotation so that $(R^{hm})^{-1} = R^{mh}$ and V_{ma} is a pure

stretch, Truesdell and Toupin [1]. The co-rotational stretching D^{km} is defined as

$$D^{km} = R^{rk} R^{nm} d_{rn} . \quad (9)$$

The linear viscoelastic deviatoric behavior can now be defined as

$$t^{km} = 2 R^{kr}(t) R^{mn}(t) \int_0^t \phi(t - \tau) D'_{rn}(\tau) d\tau , \quad (10)$$

where the function ϕ is the shear relaxation modulus. This is a special case of a more general finite strain treatment introduced by Bard [4].

— The shear relaxation modulus is taken to have the very elementary form

$$\phi(t) = G_\infty + (G_0 - G_\infty)e^{-\beta t} , \quad (11)$$

where β is a decay constant. It is customary to use a number of exponential decay terms in practice, however, the essential behavior can be demonstrated with a single term.

Creep. Creep occurs in man-made and natural materials, and in ductile materials becomes significant when the temperature on an absolute scale reaches one third to one half the material's melt temperature. It is a time dependent material mechanism in that the stress depends principally on the rate at which the material is deformed. Elastic terms are also necessary in this temperature range and are included here. In what follows the common Norton power law for secondary creep will be used, Penny and Marriott [5]. It is particularly descriptive of dislocation glide and climb deformation mechanisms in metals, Gittus [6].

It is stated in a rate form where the invariant co-rotational stress rate is related linearly to the difference between the total stretching minus the inelastic stretching d_{rs}^c . Thus,

$$\dot{\tau}_{rs} = C^{rsmn} (d_{mn} - d_{mn}^c) \quad (12)$$

where

$$d_{mn}^c = \frac{3}{2} D \left(\frac{3}{2} t'_{ij} t'^{ij} \right)^{\frac{n-1}{2}} \exp(-Q/R\theta) t'_{mn}$$

D and n are constants determined from the material, θ is absolute temperature, Q is the effective activation energy, and R is the universal gas constant.

3. EQUILIBRIUM

To handle complex loading histories, to accommodate nonlinearities from changes in geometry, and to account for inelastic material behavior, solution procedures are used which build up the solution incrementally. Terminology has been introduced which characterizes the choice of configuration where equilibrium is tested. Total Lagrangian refers to use of the reference configuration and Updated Lagrangian refers to the use of the last established equilibrium configuration. Here, the current configurations will be used to examine equilibrium. Two terminologies which are both unsatisfactory are "Eulerian" and "Updated Lagrangian + 1." The first has been used in the past in the finite element literature but has an entirely different meaning in the finite difference literature.

Equilibrium is stated in terms of the principle of virtual work.

The variational form

$$\delta\pi = \int_V t^{km} \delta x_{k,m} dv - \int_V \rho f^k \delta x_k dv - \oint_{S^1} s^k \delta x_k da \quad (13)$$

is to vanish at all points along the path of motion for all variations δx_k satisfying the displacement boundary conditions on S^2 . The integration is performed over the current configuration of the body V, where ρ is the mass density in that configuration, t^{km} is the Cauchy stress--the stress in the current configuration, and s^k is the surface traction.

Figure 2 depicts the body V in question. S^1 is that part of the surface in the current configuration acted upon by prescribed tractions and S^2 is that part of the surface in the current configuration subjected to prescribed displacements. The displacement boundary conditions are

$$x^i(x^\alpha, t) = u^i(t) \text{ on } S^2. \quad (14)$$

It is important to realize that these equations are completely general and applicable for arbitrarily large deformations.

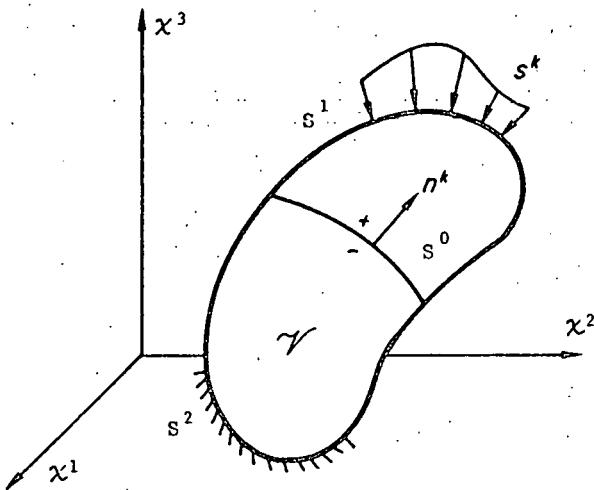


Figure 2. The body V with surface tractions s^k on the boundary S^1 and a prescribed motion on the boundary S^2 . An interior boundary S^0 with a unit normal vector n^k is pictured.

4. STRAIN INCREMENTATION

The notion of an incremental solution is fundamental to the bulk of the methods for finding a motion $x^i(x^\alpha, t)$ which generates a stress history in equilibrium with the applied loads. It is assumed that up to time t_n , the stress t_{rs} satisfies equilibrium; and the stress t_{rs}^n is the result of integrating the constitutive models with the strain histories derived from the known motion up to t_n . The prescribed loads are incremented to time t_{n+1} and a predictor/corrector method is introduced to find the new configuration $x_{n+1}^i = x^i(x^\alpha, t_{n+1})$ that has all the equilibrium properties which were deemed necessary at t_n and accuracies acceptable to the constitutive model evaluation. To indicate temporal increments a Δ is used. For example, $\Delta t = t_{n+1} - t_n$, $\Delta t_{rs} = t_{rs}^{n+1} - t_{rs}^n$, etc.

A basic assumption which underlies most incremental treatments, including the one here, but which is rarely stated is that the motion between x_n^i and x_{n+1}^i is linear. As a consequence, the incremental velocity given by $v_{n+1/2}^i = \Delta x^i / \Delta t$ is constant over the time increment. Equilibrium is tested in the configuration at t_{n+1} which is a trial configuration until equilibrium is established. To do this the stresses at t_{n+1} must be evaluated. Following Hughes and Winget [7], the one parameter family of configurations is introduced

$$x_{n+\alpha}^i = (1 - \alpha)x_n^i + \alpha x_{n+1}^i . \quad (15)$$

The gradient h_{ij} of $u_i = \Delta x^i$ with respect to $x_{n+\alpha}^j$ is given by

$$h_{ij} = \frac{\partial u_i}{\partial x_{n+\alpha}^j} \quad \text{r.c.c.} \quad (16)$$

From this gradient the strain increment e_{ij} is given by

$$e_{ij}(\alpha) = \frac{1}{2} [h_{ij} + h_{ji} + (1 - 2\alpha)h_{ki}h^k_j] \quad (17)$$

Thus, $e_{ij}(0)$ is the Green-St. Venant strain increment, $e_{ij}(1)$ is the Signorini strain increment, and

$$e_{ij}(\frac{1}{2}) = \Delta t d_{ij}^{n+1/2} = \text{sym } (u_{i,j}) . \quad (18)$$

Without the need for further linearization the configuration halfway between n and $n+1$ is selected for evaluating the stretching and the spin, and for computing Δt_{rs} . The midpoint configuration is optimal in the sense that no quadratic terms are needed to accurately evaluate $(dx^i dx_i)_{n+1} - (dx^i dx_i)_n$.

It remains to identify the strain measure which $e_{ij}(\frac{1}{2})$ approximates and establish if a satisfactory approximation of the total strain from t_0 to t_{n+1} is achieved by summing the incremental results.

Consider an infinitesimal material fiber ℓ_0 in the reference configuration which as a result of the motion $x^i(x^\alpha, t)$ has the length $\ell(t)$. If

the stretching D^{11} aligned with ℓ is evaluated and integrated in time the logarithmic strain is obtained. Thus,

$$\ln(\ell(t)/\ell_0) = \int_0^t D^{11} d\tau \quad (19)$$

If $e_{ij}(\frac{1}{2})$ is evaluated over N length changes between ℓ_0 and $\ell(t)$, the following formula is obtained:

$$\sum_{n=1}^N e_{ij}(\frac{1}{2}) \Big|_{t_{n-\frac{1}{2}}} = \sum_{n=1}^N 2 \frac{\ell_n - \ell_{n-1}}{\ell_n + \ell_{n-1}} \quad (20)$$

Table I for a range of values of the current length ℓ , lists the logarithmic strain, $e_{ij}(\frac{1}{2})$ for a one step incremental change from ℓ_0 to ℓ and the accumulated value of $e_{ij}(\frac{1}{2})$ for 2 and 10 uniform incremental changes from ℓ_0 to ℓ . The result is striking. As an approximation to $\ln(\ell/\ell_0)$, $e_{ij}(\frac{1}{2})$ is well within $\frac{1}{2}\%$ of the logarithmic strain for a $\pm 20\%$ change in ℓ_0 in one step. Summed over a series of increments, $e_{ij}(\frac{1}{2})$ rapidly converges to the logarithmic strain.

TABLE I
Midinterval extensional strain approximation for the natural strain $\ln(\ell/\ell_0)$ for $N = 1, 2$ and 10 uniform subdivisions of the change from ℓ_0 to ℓ .

ℓ/ℓ_0	$\ln(\ell/\ell_0)$	<u>$N = 1$</u>	<u>$N = 2$</u>	<u>$N = 10$</u>
.5	-0.69315	-0.66667	-0.68571	-0.69284
.6	-0.51082	-0.50000	-0.50794	-0.51071
.7	-0.35667	-0.35294	-0.35571	-0.35664
.8	-0.22314	-0.22222	-0.22291	-0.22313
.9	-0.10536	-0.10526	-0.10534	-0.10536
1.0	0.0	0.0	0.0	0.0
1.2	0.18232	0.18182	0.18219	0.18232
1.4	0.33647	0.33333	0.33566	0.33644
1.6	0.47000	0.46154	0.46777	0.46991
1.8	0.58779	0.57143	0.58333	0.58760
2.0	0.69315	0.66667	0.68571	0.69284

5. STRESS AND STATE VARIABLE ADVANCEMENT

The terms in the co-rotational derivative involving the spin w^k used in the constitutive equations (5) and (12) are for the purpose of taking into account rigid body rotations of a material point relative to the spatial coordinates x^i . In incremental form they are an orthogonal rotation through an incremental angle. Hughes and Winget [7] have provided a direct way to evaluate the incremental rotation ΔR_{ij} from the spin w_{ij} . Thus,

$$\Delta R_{ij} = (\delta_k^i - \Delta t \frac{1}{2} w_k^i)^{-1} (g_{kj} + \Delta t \frac{1}{2} w_{kj}) . \quad (21)$$

Half-angle trigonometric formulas are used to get the square-root of ΔR , $\Delta R_{ij} = \Delta R_r^{\frac{1}{2}k} \Delta R_s^{\frac{1}{2}j}$. With these constructions the constitutive models (5), (10) and (12) can be integrated over the increment from n to $n+1$. First the stress t_{rs}^n and the applicable state variables α_{rs}^n are advanced to $n + \frac{1}{2}$ by

$$\bar{t}_{rs}^{n+\frac{1}{2}} = \Delta R_r^{\frac{1}{2}i} \Delta R_s^{\frac{1}{2}j} t_{ij}^n \quad (22)$$

$$\bar{\alpha}_{rs}^{n+\frac{1}{2}} = \Delta R_r^{\frac{1}{2}i} \Delta R_s^{\frac{1}{2}j} \alpha_{ij}^n \quad (23)$$

Using $d_{rs}^{n+1/2}$ and Δt , the constitutive equations are integrated and new stresses $t_{rs}^{n+1/2}$ and state variables $\alpha_{rs}^{n+1/2}$ are obtained. These are then rotated from $n + \frac{1}{2}$ to $n + 1$ by the same process as in equations (22) and (23). Mid-interval strain and constitutive evaluation is also used by Hallquist [8] and Biffle [9].

6. INCREMENTAL CONSTITUTIVE EVALUATION

Of particular importance is the integration of the balance of the constitutive equations from time n to $n + 1$. The main requirement being to integrate the equations as accurately as possible, preferably exactly, for any Δt and stretching d_{rs} . The plasticity model is integrated from n to $n + 1$ assuming the stretching is constant which is consistent with (15). For a constant stretching path the integration is very nearly exact and is extremely reliable independent of the specific value for the time interval Δt , [10-12].

The successful implementation of the viscoelastic material rests in the recursion relation that can be developed to compute a new value of the hereditary integral at time $n + 1$ from the old value at time n . Using a direct notation to ease the profusion of sub- and superscripts, the hereditary integral at time $n + 1$ is

$$\begin{aligned}
 I_{n+1} &= R_{n+1} \int_0^{t_{n+1}} e^{-\beta(t_{n+1}-\tau)} D(\tau) d\tau R_{n+1} \\
 &= R_{n+1} \left[\int_0^{t_n} e^{-\beta(t_{n+1}-\tau)} D(\tau) d\tau \right. \\
 &\quad \left. + \int_{t_n}^{t_{n+1}} e^{-\beta(t_{n+1}-\tau)} D(\tau) d\tau \right] R_{n+1} \\
 &= \Delta R \left[e^{-\beta\Delta t} I_n + \frac{1 - e^{-\beta\Delta t}}{\beta} d(t_{n+\frac{1}{2}}) \right] \Delta R
 \end{aligned} \tag{24}$$

where ΔR is the rotation from t_n to t_{n+1} . The recursion relation provides an exact integration of a piecewise constant stretching history. The additional details needed to adapt the recursion formula to the mid-interval constitutive evaluation are omitted here. This is a special case of the work of Herrmann and Peterson [13] generalized to large deformations and finite strains.

The creep model is also integrated from n to $n + 1$ assuming the stretching is constant. The creep equations, however, are not nearly as easy to numerically integrate. They are referred to in the mathematics community as "stiff". Only with considerable effort and great expense can they be numerically integrated with conventional methods from time n to $n + 1$.

In this case, a semianalytic integration is used, [14]. Domains in stress and strain rate space are identified where various nearby differential equations with exact solutions are applicable. The solution path over a time step may remain within a single domain or may pass through two or more domains requiring the solutions to two or more of the differential equations to be applied, one after the other over the time step. In this way arbitrarily large strain or time intervals can be accurately and reliably used. An absolute maximum of seven subincrements are required so that computational time is not excessive. This approach, while conceptually straightforward is highly tailored to the constitutive model at hand.

— This approach to constitutive equations based on exact or accurate incrementation for all time steps, strains and strain rates uncouples stability and accuracy in their evaluation from the time step size used in the load incrementing schemes with their attendant equilibrium iteration, cf., Bushnell [15]. This approach contrasts with that where Δt in a constitutive integration scheme corresponds to the Δt used in incrementing the load. If this coupling is pursued, many numerical schemes can be developed. Argyris, Vaz and Willam [16] have documented a number of these and have provided the guidance necessary for their successful use.

While seemingly elaborate, these are in practice simple and quick calculations. This treatment has the property of being objective and uses a strain increment which while appearing "linear" is the same order of accuracy as using the nonlinear strain increments at either n or $n + 1$, respectively.

For examples of solved problems using these procedures references [17] and [18] can be examined.

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