Asymptotic Integration Algorithms for First-Order ODEs With Application to Viscoplasticity

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Abstract

When constructing an algorithm for the numerical integration of a differential equation, one must first convert the known ordinary differential equation (ODE), which is defined at a point, into an ordinary difference equation (OΔE), which is defined over an interval. Asymptotic, generalized, midpoint and trapezoidal, OΔE algorithms are derived for a non-linear first-order ODE written in the form of a linear ODE. The asymptotic forward (typically underdamped) and backward (typically overdamped) integrators bound these midpoint and trapezoidal integrators, which tend to cancel out unwanted numerical damping by averaging, in some sense, the forward and backward integrations.

Viscoplasticity presents itself as a system of non-linear, coupled, first-order ODEs that are mathematically stiff, and therefore difficult to numerically integrate. They are an excellent application for the asymptotic integrators. Considering a general viscoplastic structure, it is demonstrated that one can either integrate the viscoplastic stresses or their associated eigenstrains.

INTRODUCTION

This paper is composed of two parts. The first one discusses what we call asymptotic integrators, while the second one discusses their application to viscoplasticity. The purpose of this paper is to present new theoretical findings pertaining to these two topics. Numerical demonstrations are left for future papers.
Four, first-order, asymptotic integrators are presented, two of which are new. They are referred to as first-order because only the linear terms are retained in the series expansions used in their derivations. Derivations of the asymptotic forward (7) and backward (8) integrators are given in Walker and Freed (1991). From these two integrators, we obtain an asymptotic, generalized midpoint, integrator (9)—or more simply, the asymptotic midpoint integrator—which contains the asymptotic forward and backward integrators as limiting cases. The fourth integrator to be considered is an asymptotic, generalized trapezoidal, integrator (10)—or more simply, the asymptotic trapezoidal integrator—whose derivation is given in the appendix. Like the asymptotic midpoint integrator, the asymptotic trapezoidal integrator reduces to the asymptotic forward and backward integrators as limiting cases. After introducing these integrators, their asymptotic properties are discussed, and a comparison is given between them and their classical counterparts, viz. the forward and backward Euler, generalized midpoint, and generalized trapezoidal, integrators. The first part of this paper closes with a discussion on how to apply the method of Newton-Raphson iteration to update the solution for the implicit integrators.

Their are numerous viscoplastic models in the literature (see Freed et al., 1991, for a representative listing) of which the vast majority are subsets of the more general structure considered herein. The viscoplastic theory presented below is for initially isotropic materials, such as polycrystalline metals and alloys. Three types of internal stresses are considered (i.e. the back stress, the drag strength, and the yield strength) of which some or all may exist in any given viscoplastic model. Their constitutive equations, which are similar in structure to the deviatoric part of Hooke's law for an elastic/plastic material, are different in structure but equivalent in function to what one finds in the literature. This difference resides in the introduction of eigenstrains (the recovery mechanisms), they being governed by evolution equations, which in turn are functions of the viscoplastic stresses (the applied and internal stresses). Hence, one can integrate either the viscoplastic stresses or their eigenstrains, as we demonstrate. Which approach one ought to use in practice remains to be determined.

**ASYMPTOTIC INTEGRATORS**

Many physical processes, e.g. material evolution, are represented by an initial value problem (IVP) of a first-order ODE, as described by

$$\dot{X} = F [X[t]] \quad \text{given that} \quad X [0] = X_0 ,$$

where $X$ is the independent variable whose initial value at time $t = 0$ is $X_0$. This variable may be scalar, vector or tensor valued in applications. The dot $\dot{}$ is used to denote differentiation with respect to time. We choose time to be the dependent variable for illustrative purposes, as it so often is in physical applications; however, this is not a restriction on the method of numerical integration presented herein. We consider a particular subset of $F$ such that

$$F [X[t]] = C [X[t]] \left( A [X[t]] - X[t] \right) ,$$

where the time constant $C$ (a scalar herein) and the asymptote $A$ (of the same type/rank as $X$) are continuous and differentiable functions of the variable $X$. The asymptotic integrators are ideally suited for equations where $C > 0$ and $A$ is monotonic for a monotonically varying independent variable $X$, as is the case in viscoplasticity. If neither $C$ nor $A$ depends on $X$, then the equation is said to be linear; otherwise it is non-linear, as is the case in viscoplasticity.
Throughout this paper, square brackets [.] are used to denote ‘function of’, and are therefore kept logically separate from parentheses (.) and curly brackets {.} which are used for mathematical groupings.

The ODE in (1) is a point function in time. Numerical integration algorithms, however, are based on functions evaluated over an interval in time. We therefore introduce the IVP for the first-order ODE, i.e.

\[ \frac{\Delta X}{\Delta t} = \mathcal{F} [X_{n+\phi}] , \]  

where

\[ \Delta X = X_{n+1} - X_n \quad \text{with} \quad X_{n=0} = X_0 , \]

resulting in the one-step method

\[ X_{n+1} = X_n + \mathcal{F} [X_{n+\phi}] \cdot \Delta t . \]

This relationship is used to represent the IVP of the first-order ODE in numerical integration. We use the notation \( X_{n} \equiv X[t] \), \( X_{n+\phi} \equiv X[t+\phi \Delta t] \) and \( X_{n+1} \equiv X[t+\Delta t] \), where \( 0 \leq \phi \leq 1 \).

The formulation is explicit whenever \( \phi = 0 \); whereas, it is implicit whenever \( 0 < \phi \leq 1 \). Our objective is to obtain \( \mathcal{F} \) for the forward, backward, midpoint, and trapezoidal, asymptotic integrators.

One can introduce an integrating factor into the differential equation (1-2), and as a consequence obtain the recursive integral equation

\[ X[t+\Delta t] = \exp \left[ - \int_{\xi=t}^{t+\Delta t} C[X[\xi]] \, d\xi \right] X[t] + \int_{\xi=t}^{t+\Delta t} \exp \left[ - \int_{\zeta=\xi}^{t+\Delta t} C[X[\zeta]] \, d\zeta \right] C[X[\xi]] A[X[\xi]] \, d\xi , \]

which is the exact solution to this first-order ODE. John Bernoulli (1697) developed a non-recursive solution similar to (6) for the equation \( \dot{X} = aX + bX^n \), whose solution was sought earlier by Jacob Bernoulli (1695). John’s solution is expressed as a quadrature, since the integral of \( dz/z \) in the form of a logarithm was not generally known until later that same year (cf. Ince, 1956). The second line in (6) accounts for the non-homogeneous contribution to the solution. It is a Laplace (1820) integral when the integrand has its largest value at the upper limit \( t+\Delta t \), and therefore possesses an evanescent memory of the forcing function \( C[X[\xi]] A[X[\xi]] \) provided that \( C[X[\zeta]] > 0 \) over the interval \( (t, t+\Delta t) \). This fading memory means that the solution will depend mainly on the recent values of the forcing function, and that by concentrating the accuracy on the recent past we obtain accurate asymptotic representations of the solution.

Walker and Freed (1991) obtained a variety of asymptotic and exact solutions to (6) by expanding the functions \( C \) and \( A \) into series, and then integrating term by term; in particular, one obtains the first-order, asymptotic, forward integrator,

\[ X_{n+1} = e^{-C[X_n] \cdot \Delta t} X_n + \left( 1 - e^{-C[X_n] \cdot \Delta t} \right) A[X_n] , \]

and the first-order, asymptotic, backward integrator,

\[ X_{n+1} = e^{-C[X_{n+1}] \cdot \Delta t} X_n + \left( 1 - e^{-C[X_{n+1}] \cdot \Delta t} \right) A[X_{n+1}] , \]
by expanding \( C \) and \( A \) in Taylor series about the lower and upper limits of integration, respectively, and truncating them after their linear terms. Application of these integrators to perfect plasticity has been discussed by Simo and Taylor (1986), and used by Margolin and Flower (1991) who found asymptotic integration to be more accurate than the radial return algorithms. Application has also been made to viscoplasticity by Walker (1981, 1987), Ju (1990), Walker and Freed (1991), Iskovitz et al. (1991), and Freed and Walker (1992), who have shown that asymptotic integration is preferred over classical integration for viscoplastic analysis.

An asymptotic midpoint integrator (a new algorithm) is easily acquired by adding the contribution from the implicit integrator (8) taken over the interval \((t, t + \phi \Delta t)\) with that of the explicit integrator (7) taken over the remaining interval \((t + \phi \Delta t, t + \Delta t)\), resulting in

\[
X_{n+1} = e^{-C[X_{n+\phi}] \Delta t} X_n + \left(1 - e^{-C[X_{n+\phi}] \Delta t}\right) A[X_{n+\phi}], \tag{9}
\]

Whenever \( \phi = 0 \), this integrator reduces to the forward integrator (7); likewise, whenever \( \phi = 1 \), it reduces to the backward integrator (8).

The asymptotic trapezoidal integrator (another new algorithm) is obtained from the same procedure used to acquire the forward and backward integrators, except now the series expansions are weighted about both limits of integration, instead of just one. The resulting integrator is

\[
X_{n+1} = e^{-C_1[X_n, X_{n+1}] \Delta t} X_n + \frac{C_1[X_n, X_{n+1}]}{C_2[X_n, X_{n+1}]} \left(1 - e^{-C_2[X_n, X_{n+1}] \Delta t}\right) A_1[X_n, X_{n+1}], \tag{10}
\]

where

\[
A_1[X_n, X_{n+1}] = (1 - \phi)A[X_n] + \phi A[X_{n+1}], \tag{11}
\]

\[
C_1[X_n, X_{n+1}] = (1 - \phi)C[X_n] + \phi C[X_{n+1}], \tag{12}
\]

\[
C_2[X_n, X_{n+1}] = (1 - \phi)^2C[X_n] + \phi(2 - \phi)C[X_{n+1}], \tag{13}
\]

and whose derivation is given in the appendix. This integrator distinguishes itself from the prior three integrators in that it is a two-point integrator, i.e., it has a functional dependence on both \( X_n \) and \( X_{n+1} \), instead of a one-point integrator. Whenever \( \phi = 0 \), this integrator reduces to the forward integrator (7); likewise, whenever \( \phi = 1 \), it reduces to the backward integrator (8).

These four asymptotic integrators are exact and equivalent whenever \( C \) and \( A \) are both constants, i.e., whenever the ODE is linear; otherwise, they are approximations. Higher-order asymptotic integrators can be found in Walker and Freed (1991).

**Asymptotic Properties**

To acquire the asymptotic backward integrator, the integrands in (6) were expanded in Taylor series about their upper limits (Walker, 1987, and Walker and Freed, 1991), where each integrand has its largest value and contributes the most to the integral. By retaining but a single term in the Taylor series expansions, the integrands are accurately approximated where they are largest, and the neglect of the higher-order terms is only felt near the lower limits where each integrand contributes only a small amount to the integral because of its exponential decay from the upper limit. The neglect of the higher-order terms in the Taylor series thus results in an algorithm that is asymptotically correct at the upper limit; in particular, the asymptotic expansion for the backward ODE (8) is given by

\[
\lim_{\Delta t \to \text{large} \atop C > 0} X_{n+1} \propto A[X_{n+1}], \tag{14}
\]
which is the correct asymptote for the ODE in (1-2). Normally, when treating asymptotic expansions, the exponential decay of the integrand allows the lower limit to be replaced with zero or minus infinity to ease the integration. This was not done in the present case, however, so that by retaining the lower limit as \( t \), we obtain a uniformly valid asymptotic algorithm in the fully implicit approximation, provided that \( C[\mathbf{X}[\varsigma]] > 0 \) over the interval \( (t, t + \Delta t) \).

To acquire the asymptotic forward integrator, the integrands in (6) were expanded in Taylor series about their lower limits (Walker and Freed, 1991), where the neglect of the higher-order terms in the Taylor series results in integrands that become progressively more inaccurate as they approach their upper limits where the contribution from each integrand is most important. The explicit approximation is not, therefore, a valid asymptotic representation of the integral when the Taylor series is truncated at a finite number of terms. In contrast with (14), the asymptotic expansion for the forward OAE (7) is given by

\[
\lim_{\Delta t \to \text{large}} X_{n+1} \approx A[X_n],
\]

which can produce the correct asymptote for the ODE in (1-2), but only when \( A[X_n] \approx A[X_{n+1}] \); in other words, \( X_n \) must be in the neighborhood of its asymptote \( A \) in order for the asymptotic forward integrator to predict an accurate asymptotic value.

The asymptotic midpoint and trapezoidal integrators contain the forward and backward asymptotic integrators as their limits. Their respective asymptotic expansions are

\[
\lim_{\Delta t \to \text{large}} X_{n+1} \approx A[X_{n+\phi}],
\]

and

\[
\lim_{\Delta t \to \text{large}} X_{n+1} \approx \left( \frac{C_1[X_n, X_{n+1}]}{C_2[X_n, X_{n+1}]} \right) A_1[X_n, X_{n+1}],
\]

which, like the asymptotic forward integrator, can both produce the correct asymptote for the ODE in (1-2), but only when \( A[X_{n+\phi}] \approx A[X_{n+1}] \) or when \( C[X_n] \approx C[X_{n+1}] \) and \( A[X_n] \approx A[X_{n+1}] \), respectively. The asymptotic properties of these two integrators improves as \( \phi \) approaches the value of 1. Why then would one choose a value for \( \phi \) other than 1? The answer is because when \( \phi = 0 \), these integrators produce an underdamped transient response; whereas, when \( \phi = 1 \), they produce an overdamped transient response. Therefore by choosing an appropriate value for \( \phi \), which will depend on the specific ODE being integrated, one can effectively cancel out any unwanted damping in the solution that is caused by the integrator. Unfortunately, there is no known rigorous procedure for determining an optimum value for \( \phi \).

All four asymptotic integrators have the desirable property that \( \mathbf{X} \) goes to \( A \) as the ODE saturates, independent of whatever numerical error may have accumulated while integrating through the transient domain. This property is not shared by their classical counterparts. Multiple time steps are required to mitigate oscillations when integrating to saturation using \( 0 \leq \phi < 1 \); remarkably, one time step is often sufficient when integrating to saturation using \( \phi = 1 \).

**Asymptotic vs. Classical OΔEs**

Rearranging the recursive solutions of (7-10) into the form of the difference equation in (5), one obtains the one-step, asymptotic, forward integrator,

\[
\mathbf{X}_{n+1} = \mathbf{X}_n + \mathcal{F}_f[\mathbf{X}_n] \cdot \Delta t,
\]
where
\[ \mathcal{F}_f[X_n] = \left( \frac{1 - e^{-C[X_n] \cdot \Delta t}}{C[X_n] \cdot \Delta t} \right) F[X_n] \]  

(19)

de the one-step, asymptotic, backward integrator,
\[ X_{n+1} = X_n + \mathcal{F}_b[X_{n+1}] \cdot \Delta t, \]

(20)

where
\[ \mathcal{F}_b[X_{n+1}] = \left( \frac{e^{+C[X_{n+1}] \cdot \Delta t} - 1}{C[X_{n+1}] \cdot \Delta t} \right) F[X_{n+1}] \]

(21)

de the one-step, asymptotic, midpoint integrator,
\[ X_{n+1} = X_n + \mathcal{F}_\phi[X_{n+\phi}] \cdot \Delta t, \]

(22)

where
\[ \mathcal{F}_\phi[X_{n+\phi}] = \left( \frac{(1 - e^{-C[X_{n+\phi}] \cdot \Delta t})/(C[X_{n+\phi}] \cdot \Delta t)}{1 - \phi(1 - e^{-C[X_{n+\phi}] \cdot \Delta t})} \right) F[X_{n+\phi}] \]

(23)

given that
\[ X_{n+\phi} = X_n + \phi \mathcal{F}_b[X_{n+\phi}] \cdot \Delta t \]

\[ = X_n + \phi \left( \frac{e^{+C[X_{n+\phi}] \cdot \Delta t} - 1}{\phi C[X_{n+\phi}] \cdot \Delta t} \right) F[X_{n+\phi}] \cdot \Delta t \]

\[ \neq (1 - \phi)X_n + \phi X_{n+1} \quad \text{unless} \quad \phi = 1; \]

(24)

and the one-step, asymptotic, trapezoidal integrator,
\[ X_{n+1} = X_n + \mathcal{F}_t[X_n, X_{n+1}] \cdot \Delta t, \]

(25)

where
\[ \mathcal{F}_t[X_n, X_{n+1}] = C_1[X_n, X_{n+1}] \left\{ \left( \frac{1 - e^{-C_2[X_n, X_{n+1}] \cdot \Delta t}}{C_2[X_n, X_{n+1}] \cdot \Delta t} \right) A_1[X_n, X_{n+1}] \right\} \]

\[ - \left( \frac{1 - e^{-C_1[X_n, X_{n+1}] \cdot \Delta t}}{C_1[X_n, X_{n+1}] \cdot \Delta t} \right) X_n \]

(26)

which, unlike the prior \( \mathcal{F} \)s, cannot be written as a simple function of \( F \). It is easily verified that (18) and (20) are the limiting cases of (22) and (25). All four asymptotic difference functions \( \mathcal{F} \) are non-linear and have an explicit dependence on the time step size \( \Delta t \).

Contrast these asymptotic integrators with their classical counterparts; namely, the forward Euler integrator,
\[ X_{n+1} = X_n + \mathcal{F}_f[X_n] \cdot \Delta t, \]

(27)

where
\[ \mathcal{F}_f[X_n] = F[X_n] \]

(28)

de the backward Euler integrator,
\[ X_{n+1} = X_n + \mathcal{F}_b[X_{n+1}] \cdot \Delta t, \]

(29)
where

\[ \mathcal{F}_b[X_{n+1}] = F[X_{n+1}] ; \]  

(30)

the classical, generalized, midpoint integrator,

\[ X_{n+1} = X_n + \mathcal{F}_\phi[X_{n+\phi}] \cdot \Delta t , \]  

(31)

where

\[ \mathcal{F}_\phi[X_{n+\phi}] = F[X_{n+\phi}] \]  

(32)

given that

\[ X_{n+\phi} = X_n + \phi \mathcal{F}_b[X_{n+\phi}] \cdot \Delta t \]
\[ = X_n + \phi F[X_{n+\phi}] \cdot \Delta t \]
\[ = (1 - \phi)X_n + \phi X_{n+1} \quad \forall \phi ; \]  

(33)

and the classical, generalized, trapezoidal integrator,

\[ X_{n+1} = X_n + \mathcal{F}_t[X_n, X_{n+1}] \cdot \Delta t , \]  

(34)

where

\[ \mathcal{F}_t[X_n, X_{n+1}] = (1 - \phi)\mathcal{F}_f[X_n] + \phi \mathcal{F}_b[X_{n+1}] \]
\[ = (1 - \phi)F[X_n] + \phi F[X_{n+1}] . \]  

(35)

Obviously, (27) and (29) are the limiting cases of (31) and (34). Unlike their asymptotic counterparts, the classical difference functions \( \mathcal{F} \) are linear and do not have an explicit dependence on the time step size \( \Delta t \).

The classical midpoint integrator (31) is unconditionally stable over the interval \( \frac{1}{2} \leq \phi \leq 1 \); curiously, the classical trapezoidal integrator (34) is not stable at \( \phi = \frac{1}{2} \) for non-linear problems (Hughes, 1983). With respect to a local truncation error, they are second-order accurate when \( \phi = \frac{1}{2} \). Similar statements pertaining to the properties of stability and truncation error, as they apply to the asymptotic midpoint and trapezoidal integrators (22 and 25), are not presently available.

The extra terms in the asymptotic difference functions (19, 21, 23), the likes of which are not found in their classical counterparts (28, 30, 32), are the source of the asymptotic characteristics of our integrators; characteristics not shared by the classical integrators. These asymptotic integrators reduce to their classical counterparts only in the limit as \( C \Delta t \rightarrow 0 \). The asymptotic, trapezoidal, difference function (26) bears little resemblance to its classical counterpart (35).

**Midpoint Solution Procedure**

To effect the integration—via the midpoint integrators—for updating the solution from \( X_n \) to \( X_{n+1} \), one can adopt the following procedure. First, use a backward integrator (24 or 33) over the interval \( (t, t+\phi \Delta t) \) to determine \( X_{n+\phi} \). Then, use the midpoint integrator (22 or 31, respectively) over the interval \( (t, t+\Delta t) \) to determine \( X_{n+1} \). In essence, we are implicitly integrating over the interval \( (t, t+\phi \Delta t) \), and then explicitly integrating over the interval \( (t+\Delta t) \) at some midpoint \( t+\phi \Delta t \).
Applying the method of Newton-Raphson iteration to enable the implicit integration of (24 or 33) over the interval \((t, t + \phi \Delta t)\) leads to a correction \(\delta X\) for the \(i\)th iterate approximation \(X^{(i)}_{n+\phi}\) that is resolved from the linear system of equations,

\[
\left\{ I - \phi \Delta t \left( \frac{\partial F_b[X^{(i)}]}{\partial X^{(i)}_{n+\phi}} \right) \right\} \cdot \delta X = X_n + \phi F_b[X^{(i)}_{n+\phi}] \Delta t - X^{(i)}_{n+\phi},
\]

where \(I\) is the identity matrix. The next approximation is then calculated from

\[
X^{(i+1)}_{n+\phi} = X^{(i)}_{n+\phi} + \delta X,
\]

which is substituted back into (36) with iteration continuing until the convergence criterion,

\[
\|X_n + \phi F_b[X^{(i)}_{n+\phi}] \Delta t - X^{(i)}_{n+\phi}\| < e,
\]

is satisfied for some norm \(\| \cdot \|\) and maximum tolerance or error \(e\). Now that \(X_{n+\phi}\) is a known quantity, one uses the associated midpoint integrator (22 or 31) over the interval \((t, t + \Delta t)\) to update \(X_{n+1}\).

This algorithm, although appearing to be different, is equivalent to the one used by others (see, for example, Hornberger and Stamm, 1989) who, in effect, combine the implicit and midpoint integrations into the Newton-Raphson iteration. One can combine these two steps into a single one for the classical midpoint integrator, because of the linearity in (33); however, this cannot be done for the asymptotic midpoint integrator, because of the non-linearity in (24).

The derivative of \(F_b\) in (21) with respect to \(X^{(i)}_{n+\phi}\) is the Jacobian in (36) for the asymptotic midpoint integrator; it is,

\[
\frac{\partial F_b[X^{(i)}]}{\partial X^{(i)}_{n+\phi}} = \left\{ e^{+\phi C[X^{(i)}_{n+\phi}] \Delta t} \right\} C[X^{(i)}_{n+\phi}] \left( \frac{\partial A[X^{(i)}]}{\partial X^{(i)}_{n+\phi}} - I \right)
+ \left\{ e^{+\phi C[X^{(i)}_{n+\phi}] \Delta t} \right\} \frac{\partial C[X^{(i)}]}{\partial X^{(i)}_{n+\phi}} \left( A[X^{(i)}] - X^{(i)}_{n+\phi} \right),
\]

which has an explicit dependence on the time step size \(\phi \Delta t\). Similarly, from (30) one obtains the Jacobian associated with the classical midpoint integrator; it is,

\[
\frac{\partial F_b[X^{(i)}]}{\partial X^{(i)}_{n+\phi}} = C[X^{(i)}_{n+\phi}] \left( \frac{\partial A[X^{(i)}]}{\partial X^{(i)}_{n+\phi}} - I \right) + \frac{\partial C[X^{(i)}]}{\partial X^{(i)}_{n+\phi}} \left( A[X^{(i)}] - X^{(i)}_{n+\phi} \right),
\]

which contrary to (39), does not explicitly depend on the time step size \(\phi \Delta t\). The asymptotic Jacobian differs from the classical one by the coefficients found in the curly brackets of (39). Both of these Jacobians are expressed in terms of the derivatives of the time constant \(C\) and the asymptote \(A\) taken with respect to the independent variable \(X^{(i)}_{n+\phi}\).

**Trapezoidal Solution Procedure**

The updating of the solution from \(X_n\) to \(X_{n+1}\) using the trapezoidal integrators (25 or 34) can also be accomplished through Newton-Raphson iteration, where

\[
\left\{ I - \Delta t \left( \frac{\partial F_t[X_n, X^{(i)}_{n+1}]}{\partial X_{n+1}} \right) \right\} \cdot \delta X = X_n + F_t[X_n, X^{(i)}_{n+1}] \Delta t - X^{(i)}_{n+1},
\]
with the next approximation being calculated from
\[ X_{n+1}^{(i+1)} = X_{n+1}^{(i)} + \delta X \] (42)
which is substituted back into (41) and iterated upon until the convergence criterion,
\[ \| X_n + F_i[X_n, X_{n+1}^{(i)}] \cdot \Delta t - X_{n+1}^{(i)} \| < \epsilon \] (43)
is satisfied; whence, the solution is updated.

The derivative of \( F_i \) in (26) with respect to \( X_{n+1} \) is the Jacobian in (41) for the asymptotic trapezoidal integrator; it is,
\[
\frac{\partial F_i[X_n, X_{n+1}^{(i)}]}{\partial X_{n+1}} = \phi \left\{ \left( 1 - e^{-C_2[X_n, X_{n+1}^{(i)}] \cdot \Delta t} \right) \left( \frac{\partial C[X_{n+1}^{(i)}]}{\partial X_{n+1}} A_1[X_n, X_{n+1}^{(i)}] \right) + C_1[X_n, X_{n+1}^{(i)}] \frac{\partial A[X_{n+1}^{(i)}]}{\partial X_{n+1}} \right\} - e^{-C_1[X_n, X_{n+1}^{(i)}] \cdot \Delta t} \frac{\partial C[X_{n+1}^{(i)}]}{\partial X_{n+1}} X_n \\
+ \left( 2 - \phi \right) \left( \frac{1 + C_2[X_n, X_{n+1}^{(i)}] \cdot \Delta t}{(C_2[X_n, X_{n+1}^{(i)}] \cdot \Delta t)^2} e^{-C_2[X_n, X_{n+1}^{(i)}] \cdot \Delta t} - 1 \right) \\
\times C_1[X_n, X_{n+1}^{(i)}] \frac{\partial C[X_{n+1}^{(i)}]}{\partial X_{n+1}} A_1[X_n, X_{n+1}^{(i)}] \cdot \Delta t \right\}, \] (44)
which has an explicit dependence on the time step size \( \Delta t \). Similarly, from (35) one obtains the Jacobian associated with the classical trapezoidal integrator; it is,
\[
\frac{\partial F_i[X_n, X_{n+1}^{(i)}]}{\partial X_{n+1}} = \phi \left\{ C[X_{n+1}^{(i)}] \left( \frac{\partial A[X_{n+1}^{(i)}]}{\partial X_{n+1}} - I \right) + \frac{\partial C[X_{n+1}^{(i)}]}{\partial X_{n+1}} \left( A[X_{n+1}^{(i)}] - X_{n+1}^{(i)} \right) \right\}, \] (45)
which contrary to (44), does not explicitly depend on the time step size \( \Delta t \). Both of these Jacobians are expressed in terms of the derivatives of the time constant \( C \) and the asymptote \( A \) taken with respect to the independent variable \( X_{n+1} \).

**VISCOPLASTICITY**

The analysis of metallic response for high temperature applications requires mathematical models capable of accurately predicting short-term plastic strain, long-term creep strain, and the interactions between them. Viscoplastic models attempt to do that. Multiaxial, cyclic and non-isothermal loading histories are normal service conditions—not exceptional ones—all of which challenge the predictive capabilities of such models.

The stress \( \sigma_{ij} \) is taken to be related to the infinitesimal strain \( \epsilon_{ij} \) through the constitutive equations of an isotropic Hookean material, \textit{viz.}
\[ S_{ij} = 2\mu \left( E_{ij} - \epsilon_{ij}^p \right) \quad \text{where} \quad \epsilon_{ii}^p = 0, \] (46)
and
\[ \sigma_{ii} = 3\kappa \left( \epsilon_{ii} - \alpha(T - T_0)\delta_{ii} \right), \] (47)
which are characterized by the shear $\mu$ and bulk $\kappa$ elastic moduli, and where

$$S_{ij} = \sigma_{ij} - \frac{1}{3} \sigma_{kk} \delta_{ij} \quad \text{and} \quad E_{ij} = \epsilon_{ij} - \frac{1}{3} \epsilon_{kk} \delta_{ij}$$

(48)

denote the deviatoric stress and strain, respectively. The constant $\alpha$ is the mean coefficient of thermal expansion, which acts on the difference between the current temperature $T$ and some reference temperature $T_0$. The quantity $\delta_{ij}$ is the Kronecker delta; it is 1 if $i = j$, otherwise it is 0. Repeated Latin indices are summed over from 1 to 3 in the usual manner. Equation (46) characterizes the deviatoric response, while (47) characterizes the hydrostatic response. The plastic $\epsilon^p_{ij}$ and thermal $\alpha(T - T_0)\delta_{ij}$ strains are eigenstrains that represent deviations from deviatoric and hydrostatic elastic behaviors, respectively.

A typical viscoplastic model can admit any of three, phenomenological, internal, state variables; they are: i) a deviatoric back stress $B_{ij}$, ii) a drag strength $D$, and iii) a yield strength $Y$. The back stress accounts for kinematic hardening effects, while the drag and yield strengths account for isotropic hardening effects. These internal variables are described through their constitutive equations

$$B_{ij} = 2H\left(\epsilon^p_{ij} - X_{ij}\right) \quad \text{where} \quad X_{ii} = 0,$$

(49)

$$D = D_0 + h(p - \chi) \quad \text{where} \quad D_0 > 0,$$

(50)

$$Y = Y_0 + \bar{h}(p - \bar{\chi}) \quad \text{where} \quad Y_0 \geq 0,$$

(51)

and where $H$, $h$, and $\bar{h}$ are positive-valued hardening moduli; $X_{ij}$, $\chi$, and $\bar{\chi}$ are eigenstrains; $D_0$ and $Y_0$ are the annealed (minimum) values for the drag and yield strengths; and

$$p = \int_{\tau_0}^{t} \left\| \frac{\partial \epsilon^p}{\partial \tau} \right\| d\tau,$$

(52)

is the accumulation of plastic strain incurred over the loading history. Notice the similarity between the constitutive equation for stress (46) and those for internal state (49-51). In Hooke's law, the eigenstrain $\epsilon^p_{ij}$ represents a deviation from elasticity—a phenomenon called plasticity. In the constitutive equations for internal state, the eigenstrains $X_{ij}$, $\chi$, and $\bar{\chi}$ represent deviations from strain hardening—phenomena called recovery. This competition between the mechanisms of strain hardening and recovery is in accordance with Bailey's (1926) hypothesis that there is a "balance between the generation and removal of strain-hardened material" at steady state.

The eigenstrains in the constitutive equations (46, 49-51) are governed by evolution equations. In our general viscoplastic structure, the plastic strain is considered to evolve according to the Prager (1949) relation,

$$\dot{\epsilon}^p_{ij} = \frac{1}{2} \left\| \frac{S_{ij} - B_{ij}}{||S - B||} \right\|,$$

(53)

where $\frac{1}{2}(S_{ij} - B_{ij})/||S - B||$ defines the direction of plastic flow. The back stress is taken to recover according to the Armstrong and Frederick (1966)/Chaboche (1977) relation,

$$\dot{X}_{ij} = \frac{1}{2} \left( \frac{||B||}{L} \left\| \dot{\epsilon}^p \right\| + \vartheta R \right) \frac{B_{ij}}{||B||},$$

(54)

where $-\frac{1}{2}B_{ij}/||B||$ defines the direction of recovery for the back stress. Here $L > 0$ is the limiting state of back stress, $\vartheta > 0$ is typically an Arrhenius function of temperature, and
$R \geq 0$ is the thermal recovery function. The drag and yield strengths are considered to recover according to the Orowan (1947)/Ponter and Leckie (1976)/Chaboche (1977) relations,

\[
\begin{align*}
\dot{\epsilon} &= \frac{D}{\ell} \|\dot{\epsilon}\| + \vartheta \tau, \\
\dot{\chi} &= \frac{Y}{\tilde{\ell}} \|\dot{\epsilon}\| + \vartheta \tilde{\tau},
\end{align*}
\]

where $\ell > 0$ and $\tilde{\ell} > 0$ are the limit functions, and $\tau \geq 0$ and $\tilde{\tau} \geq 0$ the thermal recovery functions. In these evolution equations for the eigenstrains of internal state (54–56), the first term on the right hand side accounts for dynamic or strain-induced recovery, while the second one accounts for thermal or time-induced recovery.

The kinetic equation of evolution is taken to be governed by a Zener and Hollomon (1944) decomposition in state; that is,

\[
\|\dot{\epsilon}\| = \vartheta[T] Z \left( \left( \frac{\|S - B\| - Y}{D} \right) \right),
\]

where the Zener parameter $Z \geq 0$ is a temperature normalized magnitude for the plastic strain rate, which we assume incorporates a Bingham (1916)/Oldroyd (1947)/Prager (1949) criterion for yield. The Macauley bracket $\langle x \rangle$ has the value of 0 whenever $x \leq 0$, or the value of $x$ whenever $x \geq 0$.

The norms (or magnitudes) pertaining to the deviatoric tensors used herein are defined by

\[
\|I\| = \sqrt{\frac{1}{2} I_{ij} I_{ij}} \quad \text{and} \quad \|J\| = \sqrt{2 J_{ij} J_{ij}},
\]

where $I_{ij}$ is any deviatoric stress-like tensor, and $J_{ij}$ is any deviatoric strain-like tensor. These are the norms of von Mises (1913), where the coefficients have been chosen to scale the theory for shear.

The constitutive, evolution, and kinetic equations (49–57) become specific, thereby defining a particular viscoplastic model, when material functions for $\vartheta$, $Z$, $H$, $h$, $\tilde{h}$, $L$, $\ell$, $\tilde{\ell}$, $R$, $r$, and $\tilde{r}$ are provided.

**Asymptotic Form for Eigenstrains**

To gain a solution for this viscoplastic theory, one may numerically integrate the evolution equations for the four eigenstrains. This is accomplished by substituting the constitutive equations (46, 49–51) into their respective evolution equations (53–56), thereby obtaining

\[
\begin{align*}
\dot{\epsilon}_{ij}^p &= C^p \left( A_{ij}^p - \epsilon_{ij}^p \right), \\
\dot{X}_{ij} &= C^X \left( A_{ij}^X - X_{ij} \right), \\
\dot{\chi} &= C^X \left( A^X - \chi \right), \\
\dot{\tilde{\chi}} &= C^\tilde{X} \left( A^\tilde{X} - \tilde{\chi} \right),
\end{align*}
\]

whose time constants are given by

\[
C^p = \frac{\mu + H}{\|S - B\| \|\dot{\epsilon}\|} \geq 0,
\]

11
\[
C^x = \frac{H}{L} \| \dot{e}^p \| + \frac{H}{\| B \|} \vartheta R \geq 0, \quad (64)
\]
\[
C^x = \frac{h}{\ell} \| \dot{e}^p \| + \frac{h}{D} \vartheta r \geq 0, \quad (65)
\]
\[
C^\dot{x} = \frac{\dot{h}}{\ell} \| \dot{e}^p \| + \frac{\dot{h}}{Y} \vartheta \ddot{r} \geq 0, \quad (66)
\]

and whose asymptotes are given by

\[
A^p_{ij} = \frac{\mu}{\mu + H} E_{ij} + \frac{H}{\mu + H} X_{ij}, \quad (67)
\]
\[
A^X_{ij} = \dot{e}^p_{ij}, \quad (68)
\]
\[
A^x = \frac{D_0}{\dot{h}} + p, \quad (69)
\]
\[
A^\dot{x} = \frac{Y_0}{\ddot{h}} + p. \quad (70)
\]

These are well behaved equations for the asymptotic integrators because i) the time constants are non-negative, and ii) the asymptotes are monotonic and bounded for monotonically varying independent variables. The inequalities associated with the time constants require that \( \| \dot{e}^p \| = 0 \) when \( \| S - B \| = 0 \), that \( R = 0 \) when \( \| B \| = 0 \), and that \( \ddot{r} = 0 \) when \( Y = Y_0 = 0 \), all of which are reasonable restrictions.

\section*{Asymptotic Form for Stresses}

An alternative means of updating the solution is to integrate the viscoplastic stresses rather than their eigenstrains. This is accomplished by differentiating the constitutive equations (46, 49–51) and then combining these relations with their evolution equations (53–56), thereby resulting in the more complex system of equations

\[
\dot{S}_{ij} = C^S \left( A^S_{ij} - S_{ij} \right), \quad (71)
\]
\[
\dot{B}_{ij} = C^B \left( A^B_{ij} - B_{ij} \right), \quad (72)
\]
\[
\dot{D} = C^D \left( A^D - D \right), \quad (73)
\]
\[
\dot{Y} = C^Y \left( A^Y - Y \right), \quad (74)
\]

whose time constants are given by

\[
C^S = \frac{\mu}{\| S - B \| \| \dot{e}^p \| - \frac{\partial \mu}{\partial T} \dot{T}}, \quad (75)
\]
\[
C^B = H \left\{ \left( \frac{L + \| S - B \|}{L \| S - B \|} \right) \| \dot{e}^p \| + \frac{\vartheta R}{\| B \|} - \frac{\dot{H}}{H^2} \right\}, \quad (76)
\]
\[
C^D = \dot{h} \left( \frac{\| \dot{e}^p \|}{\ell} + \frac{\vartheta r}{D} - \frac{\dot{h}}{h^2} \right), \quad (77)
\]
\[
C^Y = \ddot{h} \left( \frac{\| \dot{e}^p \|}{\ell} + \frac{\vartheta \ddot{r}}{Y} - \frac{\ddot{h}}{h^2} \right), \quad (78)
\]
and whose asymptotes are given by

\[ A^S_{ij} = \frac{2\dot{E}_{ij} + (\|\dot{\varepsilon}^p\|/\|S - B\|)B_{ij}}{\|\dot{\varepsilon}^p\|/\|S - B\| - ((\partial\mu/\partial T)/\mu^2)\dot{T}}, \]  

\[ A^B_{ij} = \frac{(\|\dot{\varepsilon}^p\|/\|S - B\|)S_{ij}}{(\|\dot{\varepsilon}^p\|/\|S - B\|)S_{ij}} \]  

\[ A^D = \frac{\|\dot{\varepsilon}^p\|/(\dot{h}/h^2)D_0}{\|\dot{\varepsilon}^p\|/(\dot{h}/h^2)D_0 - \dot{\dot{h}}/h^2}, \]  

\[ A^Y = \frac{\|\dot{\varepsilon}^p\|/(\dot{h}/h^2)Y_0}{\|\dot{\varepsilon}^p\|/(\dot{h}/h^2)Y_0 - \dot{\dot{h}}/h^2}. \]  

These relationships account for the fact that the shear modulus \( \mu \) varies with temperature, and that the hardening moduli \( H, h, \) and \( \dot{h} \) may vary with state, as they do in some viscoplastic models; hence, their rates of change must be taken into consideration when integrating the stresses. This complexity is not present in the previous approach where the eigenstrains are integrated. Because of these rates of change in the moduli, it is possible—although not probable—that the time constants \( C \) may become negative valued, and as a consequence, the asymptotes may become unbounded. (Unlike the previous approach, here the time constants appearing in the denominators do not divide out in the equations for the asymptotes; hence, the capability of these asymptotes becoming unbounded.) Nevertheless, integrating the stresses does have one advantage over integrating the eigenstrains; that is, the asymptotes \( A^S_{ij}, A^B_{ij}, A^D, \) and \( A^Y \) become stationary at steady state; whereas, \( A^P_{ij}, A^X_{ij}, A^X, \) and \( A^X \) continue to vary at steady state. In all of our implementations of asymptotic integrators applied to viscoplastic models (Walker, 1981, 1987, Walker and Freed, 1991, and Freed and Walker, 1992), the viscoplastic stresses were always the integrated variables.

**SUMMARY**

This paper presents two, new, numerical integrators—the asymptotic midpoint and trapezoidal integrators—which contain the asymptotic forward (\( \phi = 0 \)) and backward (\( \phi = 1 \)) integrators as their limiting cases. By varying \( \phi \) between 0 and 1, one can minimize any unwanted damping in the solution that is caused by the integrator. The forward integrator is typically underdamped, while the backward integrator is typically overdamped. Which of these two, new, asymptotic integrators is preferred for applications is a subject of future work.

Viscoplasticity is an application where the asymptotic backward integrator has been used with great success. A general viscoplastic structure is presented in this paper. Into this structure we introduce a new concept referred to as the viscoplastic eigenstrains, which account for various recovery/softening mechanisms. This concept enables one to better visualize the structure of viscoplastic theory, with an added benefit of providing two options for updating/integrating the viscoplastic IVP. One may either integrate the eigenstrains or their viscoplastic stresses. Both approaches have their plus and minus points from a theoretical perspective, but whether one ought to integrate the eigenstrains or their stresses in practice is a subject of future work.
REFERENCES


APPENDIX

The derivation of the asymptotic trapezoidal integrator (10) is given below. The method of solution is: i) obtain an appropriate series expansion for the integral in the two exponentials of (6), ii) expand \( A[X[\xi]] \) and \( C[X[\xi]] \) into appropriate series expansions, and iii) analytically integrate the remaining integral—the non-homogeneous contribution—with its approximated integrand. The trapezoidal algorithm, by definition, weights the integrand at its two limits of integration.

For the first step in the solution procedure, let us consider a Taylor series expansion for an integral about its lower limit,

\[
\int_{\xi=a}^{b} f[\xi] \, d\xi = f[a](b-a) + \frac{1}{2} f'[a](b-a)^2 + \frac{1}{6} f''[a](b-a)^3 + \cdots , \tag{83}
\]

and one about its upper limit,

\[
\int_{\xi=a}^{b} f[\xi] \, d\xi = f[b](b-a) - \frac{1}{2} f'[b](b-a)^2 + \frac{1}{6} f''[b](b-a)^3 - \cdots , \tag{84}
\]

which assumes the integrand \( f \) to be continuous and differentiable over the domain \((a, b)\). Truncating these expansions after their linear term, taking \( 1-\phi \) of the lower one and \( \phi \) of the upper one, where \( 0 \leq \phi \leq 1 \), and then adding these two contributions, allows the integral in the two exponentials of (6) to be approximated as

\[
X_{n+1} \simeq e^{-((1-\phi)C[X_n] + \phi C[X_{n+1}]) \cdot \Delta t} X_n + \int_{\xi=t}^{t+\Delta t} e^{-((1-\phi)C[X[\xi]] + \phi C[X_{n+1}]) \cdot (t+\Delta t-\xi)} C[X[\xi]] A[X[\xi]] \, d\xi , \tag{85}
\]
given that the time constant $C$ is continuous and differentiable over the time domain $(t, t+\Delta t)$.

In the second step of the solution procedure, the functions $A[X[\xi]]$ and $C[X[\xi]]$ are expanded in Taylor series about $t$ and $t+\Delta t$, which bound $\xi$, and are then averaged such that

$$A[X[\xi]] = (1 - \phi) \left\{ A[X_n] + \dot{A}[X_n](\xi - t) + \frac{1}{2} \ddot{A}[X_n](\xi - t)^2 + \cdots \right\} + \phi \left\{ A[X_{n+1}] - \dot{A}[X_{n+1}](t + \Delta t - \xi) + \frac{1}{2} \ddot{A}[X_{n+1}](t + \Delta t - \xi)^2 + \cdots \right\}, \quad (86)$$

and

$$C[X[\xi]] = (1 - \phi) \left\{ C[X_n] + \dot{C}[X_n](\xi - t) + \frac{1}{2} \ddot{C}[X_n](\xi - t)^2 + \cdots \right\} + \phi \left\{ C[X_{n+1}] - \dot{C}[X_{n+1}](t + \Delta t - \xi) + \frac{1}{2} \ddot{C}[X_{n+1}](t + \Delta t - \xi)^2 + \cdots \right\}. \quad (87)$$

Truncating each expansion after its linear term enables the integrand of (85) to be further approximated as

$$X_{n+1} \approx e^{-\{(1-\phi)C[X_n] + \phi C[X_{n+1}]\}\Delta t} X_n + \left( (1 - \phi)C[X_n] + \phi C[X_{n+1}] \right) \left( (1 - \phi)A[X_n] + \phi A[X_{n+1}] \right) \times \int_{\xi = t}^{t + \Delta t} e^{-\{(1-\phi)^2C[X_n] + \phi(2-\phi)C[X_{n+1}]\}(t + \Delta t - \xi)} d\xi. \quad (88)$$

This step requires both the asymptote $A$ and the time constant $C$ to be continuous and differentiable over the time interval $(t, t+\Delta t)$.

The final step is to analytically integrate the remaining integral in (88). To do this, we introduce the change in variable $Z = t + \Delta t - \xi$, and hence rewrite (88) as

$$X_{n+1} \approx e^{-\{(1-\phi)C[X_n] + \phi C[X_{n+1}]\}\Delta t} X_n + \left( (1 - \phi)C[X_n] + \phi C[X_{n+1}] \right) \left( (1 - \phi)A[X_n] + \phi A[X_{n+1}] \right) \times \int_{Z = 0}^{\Delta t} e^{-\{(1-\phi)^2C[X_n] + \phi(2-\phi)C[X_{n+1}]\}Z} dZ, \quad (89)$$

such that upon integration one obtains

$$X_{n+1} \approx e^{-\{(1-\phi)C[X_n] + \phi C[X_{n+1}]\}\Delta t} X_n + \left( 1 - e^{-\{(1-\phi)^2C[X_n] + \phi(2-\phi)C[X_{n+1}]\}\Delta t} \right) \times \left( \frac{(1 - \phi)C[X_n] + \phi C[X_{n+1}]}{(1 - \phi)^2C[X_n] + \phi(2 - \phi)C[X_{n+1}]} \right) \left( (1 - \phi)A[X_n] + \phi A[X_{n+1}] \right), \quad (90)$$

which is the asymptotic trapezoidal integrator given in (10).
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<td>When constructing an algorithm for the numerical integration of a differential equation, one must first convert the known ordinary differential equation (ODE), which is defined at a point, into an ordinary difference equation (OAE), which is defined over an interval. Asymptotic, generalized, midpoint and trapezoidal, OAE algorithms are derived for a non-linear first-order ODE written in the form of a linear ODE. The asymptotic forward (typically underdamped) and backward (typically overdamped) integrators bound these midpoint and trapezoidal integrators, which tend to cancel out unwanted numerical damping by averaging, in some sense, the forward and backward integrations. Viscoplasticity presents itself as a system of non-linear, coupled, first-order ODEs that are mathematically stiff, and therefore difficult to numerically integrate. They are an excellent application for the asymptotic integrators. Considering a general viscoplastic structure, it is demonstrated that one can either integrate the viscoplastic stresses or their associated eigenstrains.</td>
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