An U-ALE formulation of 3-D unsteady viscoelastic flow

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AN U-ALE FORMULATION OF 3-D UNSTEADY VISCOELASTIC FLOW

FRANK P. T. BAAIJENS

Philips Research Laboratories, P. O. Box 80000, 5600 JA Eindhoven, The Netherlands

and

*Eindhoven University of Technology, Faculty of Mechanical Engineering, Section of Engineering Fundamentals,
P.O. Box 513, 5600 MB Eindhoven, The Netherlands*

SUMMARY

The Arbitrary-Lagrange–Euler (ALE) formulation is applied to the analysis of unsteady viscoelastic flow of an Upper-Convected-Maxwell (UCM) medium. It is shown how the requirement of *incremental objectivity* affects the stress updating scheme. The current implementation of the ALE formulation uses the Time-Discontinuous/Galerkin-Least-Squares (TD/GLS) method to handle the advective parts of the equations. Further, the ALE formulation is compared with an Updated-ALE formulation that is shown to give comparable results but is much more cost effective. The technique presented is particularly effective for free surface flows. Three applications are given.

INTRODUCTION

The numerical analysis of the flow of viscoelastic materials is a very challenging problem. This paper investigates two issues involved in these simulations.

First of all, the numerical integration in time of the constitutive equation in the unsteady case is addressed. Commonly employed integration algorithms do not preserve objectivity, carefully introduced by the use of objective rates. After introduction of the concept of *incremental objectivity*, it is shown, following Simo and Hughes,¹⁷ how the numerical approximation can be made incrementally objective for a variety of objective rates in a displacement oriented Lagrange type of formulation. Recall, by the way, that most algorithms in use nowadays to analyse viscoelastic flows employ a velocity oriented formulation in a Eulerian setting. In that case, it is not clear how to achieve incremental objectivity.

Secondly, if free surface flows occur, the Eulerian formulation usually employed is not the most appropriate approach. In such cases, the Arbitrary-Lagrange–Euler (ALE) formulation appears to be a suitable alternative, see e.g. Schreurs *et al.*,¹⁵ Liu *et al.*,¹³ Keunings,¹² Huetink *et al.*,⁹ Ghosh and Kikuchi⁷ and Soulaïmani *et al.*¹⁸ In this formulation the computational reference grid is allowed to move independently of the material, and can be selected to follow free surfaces accurately.

Two strategies to implement the ALE approach are discussed. First of all, the regular method in which the material points and grid points are updated simultaneously, and, secondly, an updated approach are discussed. In this updated technique the grid points are adjusted only *after* each time step to constitute a new configuration for the next time step. The latter approach substantially saves computing time while giving comparable results. The first technique is used

by, for instance, Schreurs *et al.*¹⁵ and Ghosh and Kikuchi,⁷ while the second approach is reported by Huetink *et al.*,⁹ but comparisons have not been made previously.

Another feature that sets the current implementation apart from others is the use of the Time-Discontinuous/Galerkin-Least-Squares (TD/GLS) (see e.g. Shakib¹⁶) formulation to handle the advective parts involved in the governing set of equations.

The structure of the paper is as follows. First of all, some aspects of the finite deformation theory are recalled. Motions and gradients of motion are reviewed. In order to define constitutive equations for arbitrary large motions properly, the concept of objectivity is briefly discussed. To satisfy objectivity principles, objective rates are presented. Actual solutions are, in the approximated sense, determined at a finite number of time points. The stress integration algorithm is selected to satisfy the concept of 'incremental objectivity'. The proposed algorithm is applied to the Upper-Convected-Maxwell (UCM) model. A precise definition of the problem and the algorithmic structure is given next. After a discussion of issues related to the Newton-Raphson iteration process, some implementation aspects and the contact conditions are reviewed. Finally, the methodology is illustrated with a number of examples.

KINEMATICS

Reference systems

To describe the kinematics of a deforming body, two reference systems are introduced. First of all, the classical Material Reference System (MRS) is defined. With this reference system the position of a *material* point (particle) can be identified and is denoted by $\mathbf{x}$. Secondly, it will be shown to be advantageous for computational purposes to introduce the so-called Computational Reference System (CRS), see e.g. Schreurs *et al.*¹⁵ A point of the CRS is called a *grid* point and its position is identified by $\mathbf{x}_g$. The motion of the grid points may be chosen independently of the motion of the material points.

Motion

Let $S = [0, T] \subset \mathbb{R}_+$ be the time interval of interest. For all $t \in [0, T]$, the mapping

$$\boldsymbol{\varphi}: \Omega_0 \subset \mathbb{R}^3 \mapsto \Omega \subset \mathbb{R}^3 \quad (1)$$

is a motion that maps the reference configuration Ω_0 onto the current configuration Ω . The reference configuration is chosen at some time $t_0 \in [0, T]$, for instance $t_0 = 0$ is suitable. The current configuration Ω is viewed as a collection of material points. This domain has boundary Γ .

A particle with position $\mathbf{x}_0 \in \Omega_0$ at time $t = t_0$ has position

$$\mathbf{x} = \boldsymbol{\varphi}(\mathbf{x}_0, t) \quad (2)$$

at time t . The explicit dependence of $\boldsymbol{\varphi}$ on $\mathbf{x}_0$ and t is often not mentioned.

The velocity of the particle identified with its reference position $\mathbf{x}_0$ is defined as

$$\mathbf{v} = \frac{\partial \boldsymbol{\varphi}(\mathbf{x}_0, t)}{\partial t} \quad (3)$$

Likewise, the motion of the grid points can be described, e.g.

$$\mathbf{x}_g = \boldsymbol{\varphi}_g(\mathbf{x}_{g0}, t), \boldsymbol{\varphi}_g: \Omega_{g0} \subset \mathbb{R}^3 \mapsto \Omega_g \subset \mathbb{R}^3 \quad (4)$$

where $\mathbf{x}_{g0}$ denotes the position of the grid point in the grid reference configuration Ω_{g0} . The

domain Ω_g is considered to be the collection of grid points that constitute the CRS and has boundary Γ_g . Clearly, the velocity of a grid point is defined by

$$\mathbf{v}_g = \frac{\partial \boldsymbol{\varphi}_g(\mathbf{x}_0, t)}{\partial t} \quad (5)$$

Deformations and rates of deformations

The deformation tensor $\mathbf{F}$ is defined as

$$\mathbf{F}(\mathbf{x}_0, t) = (\mathbf{V}_0 \boldsymbol{\varphi})^c = \frac{\partial \boldsymbol{\varphi}}{\partial \mathbf{x}_0} \quad (6)$$

The right Cauchy–Green tensor is defined as

$$\mathbf{C} = \mathbf{F}^c \cdot \mathbf{F} \quad (7)$$

Recall that the polar decomposition is defined as

$$\mathbf{F} = \mathbf{R} \cdot \mathbf{U} \quad \text{with} \quad \mathbf{U} = \mathbf{C}^{1/2} \quad (8)$$

The material time derivative of $\mathbf{F}$ is defined as

$$\dot{\mathbf{F}} = \frac{\partial \mathbf{F}(\mathbf{x}_0, t)}{\partial t} \quad (9)$$

$$= (\mathbf{V}_0 \mathbf{v})^c \quad (10)$$

As $\mathbf{V}_0 = \mathbf{F}^c \cdot \mathbf{V}$, it follows that

$$\dot{\mathbf{F}} = (\mathbf{V} \mathbf{v})^c \cdot \mathbf{F} \quad (11)$$

The velocity gradient tensor is defined as

$$\mathbf{L} = (\mathbf{V} \mathbf{v})^c = \dot{\mathbf{F}} \cdot \mathbf{F}^{-1} \quad (12)$$

The symmetric part of $\mathbf{L}$ is called the deformation rate tensor

$$\mathbf{D} = \frac{1}{2}((\mathbf{V} \mathbf{v})^c + \mathbf{V} \mathbf{v}) \quad (13)$$

while the skew-symmetric part is named the spin tensor

$$\boldsymbol{\Omega} = \frac{1}{2}((\mathbf{V} \mathbf{v})^c - \mathbf{V} \mathbf{v}) \quad (14)$$

A relation that proves to be very useful for future purposes is

$$\dot{\mathbf{C}} = 2\mathbf{F}^c \cdot \mathbf{D} \cdot \mathbf{F} \quad (15)$$

The deformation of the grid can be described similarly, resulting in a deformation tensor $\mathbf{F}_g$, a right Cauchy–Green strain tensor $\mathbf{C}_g$, etc.

Relation between MRS and CRS related quantities

Physical variables are usually associated with material points. However, if the CRS is taken as the reference system, it is necessary to relate MRS oriented quantities, such as stresses, to the grid points.

Figure 1. Relation between CRS and MRS change of a

Assume that at some time, say $t = t_n$, a grid point $\mathbf{x}_g$ coincides with material point $\mathbf{x}$, that is $\mathbf{x}_n \stackrel{\text{def}}{=} \mathbf{x}(\mathbf{x}_0, t_n) = \mathbf{x}_{gn} \stackrel{\text{def}}{=} \mathbf{x}_g(\mathbf{x}_{g0}, t_n)$. At some time $t = t_{n+1} > t_n$, the position of the grid point has changed to $\mathbf{x}_g + \Delta_g \mathbf{x}_g$, while the material point is located at $\mathbf{x} + \Delta_m \mathbf{x}$. This is illustrated in Figure 1. Now, let a be some material associated quantity; then the change of a during the state transition $t_n \rightarrow t_{n+1}$ while keeping the material point fixed, is denoted by $\Delta_m a$. The change of a with respect to the grid point that at $t = t_n$ coincided with this material point can be written as¹⁵

$$\Delta_g a = \Delta_m a + (\Delta_g \mathbf{x}_g - \Delta_m \mathbf{x}) \cdot \nabla a \quad (16)$$

This may also be expressed in terms of rates:

$$\frac{\delta a}{\delta t} = \dot{a} + (\mathbf{v}_g - \mathbf{v}) \cdot \nabla a \quad (17)$$

where $\delta a / \delta t$ denotes the grid rate of a , and $\dot{a}$ the material rate of a .

OBJECTIVITY AND OBJECTIVE RATES

For viscoelastic materials, constitutive models of the differential type are frequently used. If finite deformations occur, objective rates must be employed. Most of the objective rates in use have a common mathematical structure. The purpose of this section is to recall a theorem that describes a large class of objective rates. This theorem is used as a basis to derive objectivity-preserving numerical integration algorithms for rate-type constitutive equations.

Objectivity and invariance

Consider a motion ϕ and a superposed rigid body motion characterized by

$$\mathbf{x} \in \Omega \mapsto \mathbf{x}^+ = \mathbf{c}(t) + \mathbf{Q}(t) \cdot \mathbf{x} \quad (18)$$

where $\mathbf{c}(t)$ is a rigid body translation and $\mathbf{Q}(t)$ an orthogonal mapping, i.e. $\mathbf{Q}^c \cdot \mathbf{Q} = \mathbf{I}$, $\det(\mathbf{Q}) = 1$. Both $\mathbf{c}$ and $\mathbf{Q}$ are a function of time only.

Definition 1. A tensor $\mathbf{A}$ that, under the above superimposed rigid body motion, transforms according to

$$\mathbf{A}^+ = \mathbf{Q} \cdot \mathbf{A} \cdot \mathbf{Q}^c \quad (19)$$

is called an *objective* tensor.

Definition 2. A tensor $\mathbf{B}$ that remains unaltered under the superimposed rigid body motion, i.e.

$$\mathbf{B}^+ = \mathbf{B} \quad (20)$$

is called *invariant*.

Objective rates

A key problem in the definition of non-linear constitutive equations is the non-objectivity of the material derivative of the Cauchy stress tensor. The material derivative of the σ^+ follows from

$$\dot{\sigma}^+ = \dot{\mathbf{Q}} \cdot \sigma \cdot \mathbf{Q}^c + \mathbf{Q} \cdot \dot{\sigma} \cdot \mathbf{Q}^c + \mathbf{Q} \cdot \sigma \cdot \dot{\mathbf{Q}}^c \quad (21)$$

which is clearly non-objective.

One can construct rates that preserve objectivity by the following fundamental theorem, after van Wijngaarden and Veldpaus.¹⁹

Theorem 1. With each objective tensor σ an invariant tensor $\bar{\sigma}$ can be associated such that

$$\bar{\sigma} = \mathbf{A} \cdot \sigma \cdot \mathbf{A}^c \quad (22)$$

where $\mathbf{A}$ is defined by the initial value problem

$$\dot{\mathbf{A}} = -\mathbf{A} \cdot (\boldsymbol{\Omega} + \mathbf{H}), \quad \mathbf{A}(t = \tau) = \mathbf{I} \quad (23)$$

where τ is some reference time. The material time derivative of $\bar{\sigma}$ is associated with a so-called *objective rate* via the relations

$$\dot{\bar{\sigma}} = \mathbf{A} \cdot \overset{\diamond}{\sigma} \cdot \mathbf{A}^c \quad (24)$$

$$\overset{\diamond}{\sigma} = \dot{\sigma} - (\boldsymbol{\Omega} + \mathbf{H}) \cdot \sigma - \sigma \cdot (\boldsymbol{\Omega} + \mathbf{H})^c \quad (25)$$

where $\mathbf{H}$ is some objective tensor, and $\overset{\diamond}{\sigma}$ denotes some objective rate of σ .

Proof.

1. First it is shown that $\bar{\sigma}$ is indeed invariant. Clearly, it holds that

$$\boldsymbol{\Omega}^+ = \dot{\mathbf{Q}} \cdot \mathbf{Q}^c + \mathbf{Q} \cdot \boldsymbol{\Omega} \cdot \mathbf{Q}^c \quad (26)$$

$$\mathbf{H}^+ = \mathbf{Q} \cdot \mathbf{H} \cdot \mathbf{Q}^c \quad (27)$$

It can be shown that

$$(\dot{\mathbf{A}}^+ \cdot \mathbf{Q}) = -(\mathbf{A}^+ \cdot \mathbf{Q}) \cdot (\boldsymbol{\Omega} + \mathbf{H}) - \mathbf{A}^+ \cdot \dot{\mathbf{Q}} \quad \forall \mathbf{Q} \quad (28)$$

This can hold only for

$$\mathbf{A}^+ = \mathbf{A} \cdot \mathbf{Q}^c \quad (29)$$

This proves the invariance of $\bar{\sigma}$.

2. Secondly, it is shown that the time derivative $\overset{\diamond}{\sigma}$ is indeed an objective time derivative in the sense that, upon imposing a rigid motion on the regular motion as before, it should hold that

$$\overset{\diamond}{\sigma}^+ = \mathbf{Q}(t) \cdot \overset{\diamond}{\sigma} \cdot \mathbf{Q}(t)^c \quad (30)$$

As by definition

$$\sigma^+ = Q \cdot \sigma \cdot Q^c \quad (31)$$

it follows directly that

$$\dot{\sigma}^+ = \dot{\sigma}^+ - (\Omega^+ + H^+) \cdot \sigma^+ - \sigma^+ \cdot (\Omega^+ + H^+)^c \quad (32)$$

Using the definition of σ^+ , Ω^+ and H^+ gives

$$\dot{\sigma}^+ = Q \cdot \dot{\sigma} \cdot Q^c - Q \cdot (\Omega + H) \cdot \sigma \cdot Q^c - Q \cdot \sigma \cdot (\Omega + H)^c \cdot Q^c \quad (33)$$

which proves objectivity.

3. Employing the definition of A , it follows immediately that

$$\dot{\sigma} = \dot{A} \cdot \sigma \cdot A^c + A \cdot \dot{\sigma} \cdot A^c + A \cdot \sigma \cdot \dot{A}^c \quad (34)$$

$$= -A \cdot (\Omega + H) \cdot \sigma \cdot A^c + A \cdot \dot{\sigma} \cdot A^c - A \cdot \sigma \cdot (\Omega + H)^c \cdot A^c \quad (35)$$

$$= A \cdot \dot{\sigma} \cdot A^c \quad (36)$$

which concludes the proof.

Clearly, there are two ways to obtain objective rates: either the objective tensor H must be defined or the tensor A that satisfies equation (24) must be given. Examples are:

1. $H = 0$: Jaumann rate

$$\dot{\sigma}^\diamond = \dot{\sigma} - \Omega \cdot \sigma - \sigma \cdot \Omega^c \quad (37)$$

2. $H = D \Leftrightarrow A = F^{-1}$: Truesdell rate

$$\dot{\sigma}^\diamond = \dot{\sigma} - L \cdot \sigma - \sigma \cdot L^c \quad (38)$$

3. $H = -D \Leftrightarrow A = F^c$: Cotter-Rivlin rate

$$\dot{\sigma}^\diamond = \dot{\sigma} + L^c \cdot \sigma + \sigma \cdot L \quad (39)$$

4. $A = R^c$

$$\dot{\sigma}^\diamond = \dot{\sigma} - (\dot{R} \cdot R^c) \cdot \sigma - \sigma \cdot (\dot{R} \cdot R^c)^c \quad (40)$$

CONSTITUTIVE MODEL

The objective rates defined above apply to many constitutive equations in use nowadays. Assume the Cauchy stress tensor to be split in the common way

$$\sigma = -pI + \tau \quad (41)$$

One of the most well known classes of models are the Maxwell-type models

$$\dot{\tau}^\diamond + \frac{1}{\theta} \tau = \frac{2\eta}{\theta} D \quad (42)$$

where θ is a time constant and η a viscosity. Studies in two dimensional flow show that this model has unfavourable properties from a numerical point of view, see e.g. Baaijens.¹ The objectivity preserving numerical integration of this class of models is discussed in the next section.

The numerical integration of other models such as the Phan–Thien/Tanner (PTT) model

$$\overset{\nabla}{\boldsymbol{\tau}} + \left(\frac{1}{\theta} + \frac{\varepsilon}{\eta} \text{tr}(\boldsymbol{\tau}) \right) \boldsymbol{\tau} = 2 \frac{\eta}{\theta} \mathbf{D} \quad (43)$$

where $(\overset{\nabla}{\cdot})$ denotes the Truesdell rate, or the Giesekus model

$$\overset{\nabla}{\boldsymbol{\tau}} + \frac{1}{\theta} \boldsymbol{\tau} - \frac{\varepsilon}{\eta} \boldsymbol{\tau} \cdot \boldsymbol{\tau} = \frac{2\eta}{\theta} \mathbf{D} \quad (44)$$

or the Leonov model

$$\boldsymbol{\tau} = \frac{\eta}{\theta} \mathbf{B}_e, \quad \overset{\nabla}{\mathbf{B}}_e = -\frac{1}{2\theta} \left(\mathbf{B}_e \cdot \mathbf{B}_e - \mathbf{I} - \frac{1}{3} (\text{tr}(\mathbf{B}_e) - \text{tr}(\mathbf{B}_e^{-1})) \right) \mathbf{B}_e \quad (45)$$

can be treated likewise.

OBJECTIVE INTEGRATION OF RATE-TYPE CONSTITUTIVE EQUATIONS

In the solution schemes commonly employed, the time domain $S = [0, T]$ is split into N_t time steps

$$S = \bigcup_{n=1}^{N_t} S_n, \quad S_n = [t_n, t_{n+1}], \quad \Delta t = t_{n+1} - t_n \quad (46)$$

A time step of this kind is often referred to as an increment.

Assuming the motion to be known at the beginning and at the end of a time step S_n , a key problem is to calculate the stress state at $t = t_{n+1}$ properly. In particular, objectivity, carefully introduced through the concept of objective rates, should be preserved. This is not a trivial matter, and is mostly ignored and violated, see e.g. Fortin and Esselaoui⁴ and Fortin and Fortin.⁵ The results presented next are obtained by following Simo and Hughes.¹⁷

Let $\boldsymbol{\varphi}_n = \boldsymbol{\varphi}(\mathbf{x}_0, t_n)$ and $\boldsymbol{\varphi}_{n+1} = \boldsymbol{\varphi}(\mathbf{x}_0, t_{n+1})$ be known. One of the key assumptions employed in the sequel is that the motion of a point labelled $\mathbf{x}_0$ for $t \in S_n$ is assumed to be linearized by

$$\boldsymbol{\varphi}_{n+\alpha} = (1 - \alpha)\boldsymbol{\varphi}_n + \alpha\boldsymbol{\varphi}_{n+1}, \quad \alpha = \frac{t - t_n}{\Delta t} \in [0, 1] \quad (47)$$

So, the deformation tensor in S_n is given by

$$\mathbf{F}_{n+\alpha} = (\mathbf{V}_0 \boldsymbol{\varphi}_{n+\alpha})^c \quad (48)$$

$$= (1 - \alpha)\mathbf{F}_n + \alpha\mathbf{F}_{n+1} \quad (49)$$

For further purposes, define

$$\boldsymbol{\Lambda}_{n+\alpha} \stackrel{\text{def}}{=} \mathbf{F}_{n+\alpha} \cdot \mathbf{F}_n^{-1} \quad (50)$$

which can be interpreted as the deformation tensor that relates $\boldsymbol{\Omega}_{n+\alpha}$ to $\boldsymbol{\Omega}_n$.

For rate-type constitutive equations of the form already given, two items must be investigated. The constitutive equations cannot be integrated exactly and some numerical scheme must be chosen. The discrete approximations (in time) must be taken such that both the rate of strain tensor and the objective rate are approximated (in the discrete sense) objectively.

Definition 3. Consider a superimposed rigid body motion

$$\mathbf{x}_{n+\alpha}^+ = \mathbf{c} + \mathbf{Q} \cdot \mathbf{x}_{n+\alpha} \quad (51)$$

with a constant $\mathbf{Q}$ for $t \in S_n$. A discrete approximation of an objective tensor $\mathbf{A}$, $\mathbf{A}_{n+\alpha}$, is called *incrementally objective* if upon superposition of the above rigid body motion $\mathbf{A}_{n+\alpha}$ transforms according to

$$\mathbf{A}_{n+\alpha}^+ = \mathbf{Q} \cdot \mathbf{A}_{n+\alpha} \cdot \mathbf{Q}^c \quad \forall \alpha \in [0, 1] \quad (52)$$

Objective approximation of rate of strain tensor

Proposition 1. An incrementally objective approximation for the rate of strain tensor in S_n is given by

$$\mathbf{D}_{n+\alpha} = \frac{1}{\Delta t} \mathbf{\Lambda}_{n+\alpha}^{-c} \cdot \mathbf{E}_{n+1} \cdot \mathbf{\Lambda}_{n+\alpha}^{-1} \quad (53)$$

$$\mathbf{E}_{n+1} = \frac{1}{2} [\mathbf{\Lambda}_{n+1}^c \cdot \mathbf{\Lambda}_{n+1} - \mathbf{I}] \quad (54)$$

for all $\alpha \in [0, 1]$.

Equation (54) can be interpreted as the Green–Lagrange strain tensor of $\Omega_{n+\alpha}$ with respect to Ω_n .

Proof. The proof consists of two parts. First it is shown that equations (53) and (54) indeed hold. Thereafter, the objectivity of the algorithm is proved.

Step 1. Recall that

$$\dot{\mathbf{C}} = 2\mathbf{F}^c \cdot \mathbf{D} \cdot \mathbf{F} \quad (55)$$

Clearly,

$$\dot{\mathbf{C}}_{n+\alpha} = 2\mathbf{F}_{n+\alpha}^c \cdot \mathbf{D}_{n+\alpha} \cdot \mathbf{F}_{n+\alpha} \quad (56)$$

Application of the generalized midpoint rule gives

$$\mathbf{C}_{n+1} - \mathbf{C}_n = \dot{\mathbf{C}}_{n+\alpha} \Delta t \quad (57)$$

Recall that

$$\mathbf{F}_{n+1} = \mathbf{\Lambda}_{n+1} \cdot \mathbf{F}_n \quad (58)$$

Hence

$$\mathbf{C}_{n+1} = \mathbf{F}_{n+1}^c \cdot \mathbf{F}_{n+1} = \mathbf{F}_n^c \cdot [\mathbf{\Lambda}_{n+1}^c \cdot \mathbf{\Lambda}_{n+1}] \cdot \mathbf{F}_n \quad (59)$$

Combination of equations (57) and (59) thus yields

$$\dot{\mathbf{C}}_{n+\alpha} \Delta t = \mathbf{F}_n^c \cdot [\mathbf{\Lambda}_{n+1}^c \cdot \mathbf{\Lambda}_{n+1} - \mathbf{I}] \cdot \mathbf{F}_n \quad (60)$$

Hence

$$\mathbf{D}_{n+\alpha} = \frac{1}{\Delta t} \underbrace{\mathbf{F}_{n+\alpha}^{-c} \cdot \mathbf{F}_n^c}_{\mathbf{\Lambda}_{n+\alpha}^{-c}} \cdot \underbrace{\frac{1}{2} (\mathbf{\Lambda}_{n+1}^c \cdot \mathbf{\Lambda}_{n+1} - \mathbf{I})}_{\mathbf{E}_{n+1}} \cdot \underbrace{\mathbf{F}_n \cdot \mathbf{F}_{n+\alpha}^{-1}}_{\mathbf{\Lambda}_{n+\alpha}^{-1}} \quad (61)$$

which provides the desired result.

Step 2. To prove objectivity, consider, as before, the superposed rigid body motion

$$\mathbf{x}_{n+\alpha}^+ = \mathbf{c}(t) + \mathbf{Q} \cdot \mathbf{x}_{n+\alpha} \quad (62)$$

Clearly

$$\mathbf{F}_{n+1}^+ = \mathbf{Q} \cdot \mathbf{F}_{n+1}, \quad \mathbf{F}_n^+ = \mathbf{Q} \cdot \mathbf{F}_n \quad (63)$$

and

$$\mathbf{A}_{n+\alpha}^+ = \mathbf{Q} \cdot \mathbf{A}_{n+\alpha} \cdot \mathbf{Q}^c \quad (64)$$

Hence

$$\mathbf{E}_{n+1}^+ = \mathbf{Q} \cdot \mathbf{E}_{n+1} \cdot \mathbf{Q}^c \quad (65)$$

and

$$\mathbf{D}_{n+\alpha}^+ = \frac{1}{\Delta t} \mathbf{Q} \cdot \mathbf{A}_{n+\alpha}^{-c} \cdot \mathbf{E}_{n+1} \cdot \mathbf{A}_{n+\alpha}^{-1} \cdot \mathbf{Q}^c \quad (66)$$

This completes the proof.

Objective integration of stress rate

Proposition 2. The algorithm

$$\diamond \tau_{n+\alpha} = \frac{1}{\Delta t} \mathbf{A}_{n+\alpha}^{-1} \cdot [\mathbf{A}_{n+1} \cdot \tau_{n+1} \cdot \mathbf{A}_{n+1}^c - \mathbf{A}_n \cdot \tau_n \cdot \mathbf{A}_n^c] \cdot \mathbf{A}_{n+\alpha}^{-c} \quad (67)$$

is incrementally objective for all $\alpha \in [0, 1]$.

Proof. The algorithm follows directly from the definition of the invariant tensor associated with the objective rate:

$$\dot{\bar{\tau}}_{n+\alpha} = \frac{1}{\Delta t} (\bar{\tau}_{n+1} - \bar{\tau}_n) \quad (68)$$

$$= \frac{1}{\Delta t} (\mathbf{A}_{n+1} \cdot \tau_{n+1} \cdot \mathbf{A}_{n+1}^c - \mathbf{A}_n \cdot \tau_n \cdot \mathbf{A}_n^c) \quad (69)$$

$$= \mathbf{A}_{n+\alpha} \cdot \diamond \tau_{n+\alpha} \cdot \mathbf{A}_{n+\alpha}^c \quad (70)$$

To prove objectivity of the algorithm, it is first shown that, upon superposition of the rigid body motion equation (51), $\mathbf{A}_{n+\alpha}$ transforms according to

$$\mathbf{A}_{n+\alpha}^+ = \mathbf{A}_{n+\alpha} \cdot \mathbf{Q}^c \quad (71)$$

The subscript $n + \alpha$ is omitted for notational convenience. The above equation implies that

$$\dot{\mathbf{A}}^+ = \dot{\mathbf{A}} \cdot \mathbf{Q}^c + \mathbf{A} \cdot \dot{\mathbf{Q}}^c \quad (72)$$

$$= -\mathbf{A} \cdot (\boldsymbol{\Omega} + \mathbf{H}) \cdot \mathbf{Q}^c - \mathbf{A} \cdot \mathbf{Q}^c \cdot \dot{\mathbf{Q}} \cdot \mathbf{Q}^c \quad (73)$$

where $\dot{\mathbf{Q}} \cdot \mathbf{Q}^c + \mathbf{Q} \cdot \dot{\mathbf{Q}}^c = \mathbf{0}$ is used. At the same time, by application of the definition of $\mathbf{A}$,

equation (23), it follows that

$$\dot{\mathbf{A}}^+ = -\mathbf{A}^+ \cdot (\boldsymbol{\Omega}^+ + \mathbf{H}^+) \quad (74)$$

$$= -\mathbf{A}^+ \cdot (\dot{\mathbf{Q}} \cdot \mathbf{Q}^c + \mathbf{Q} \cdot \boldsymbol{\Omega} \cdot \mathbf{Q}^c + \mathbf{Q} \cdot \mathbf{H} \cdot \mathbf{Q}^c) \quad (75)$$

Equation (75) equals equation (73) if $\mathbf{A}$ indeed transforms according to equation (71).

The objectivity of the algorithm is shown as follows. Consider the rigid body motion as before. Then

$$\hat{\tau}_{n+\alpha}^+ = \frac{1}{\Delta t} \mathbf{Q} \cdot \mathbf{A}_{n+\alpha}^{-1} \cdot [\mathbf{A}_{n+1} \cdot \mathbf{Q}^c \cdot \mathbf{Q} \cdot \tau_{n+1} \cdot \mathbf{Q}^c \cdot \mathbf{Q} \cdot \mathbf{A}_{n+1}^c - \mathbf{A}_n \cdot \mathbf{Q}^c \cdot \mathbf{Q} \cdot \tau_n \cdot \mathbf{Q}^c \cdot \mathbf{Q} \cdot \mathbf{A}_n^c] \cdot \mathbf{A}_{n+\alpha}^{-c} \cdot \mathbf{Q}^c \quad (76)$$

$$= \mathbf{Q} \cdot \hat{\tau}_{n+\alpha} \cdot \mathbf{Q}^c \quad (77)$$

This proves the result.

Remark. In a Eulerian formulation, with velocities as the primary unknowns, the above results are *not* easily generalized. In fact, there does not seem to be an objective integration scheme available in such a formulation. The key problem is, that, given a velocity field $\mathbf{v}(\mathbf{x}, t)$, the tensor $\mathbf{A}$ of equation (23) must be calculated such that $\mathbf{A}$ has the property

$$\mathbf{A}_{n+\alpha}^+ = \mathbf{A}_{n+\alpha} \cdot \mathbf{Q}^c \quad (78)$$

This requirement is not easily satisfied. In the Appendix it is shown for the Truesdell rate that commonly applied integration rules do not preserve objectivity in a satisfactory way.

Objective integration of the UCM model

For the Truesdell rate, $\mathbf{A} = \mathbf{F}^{-1}$, hence within time step S_n the Upper-Convected-Maxwell (UCM) model can be approximated by using equations (53), (54) and (67), giving

$$\begin{aligned} & \frac{1}{\Delta t} \mathbf{F}_{n+\alpha} \cdot [\mathbf{F}_{n+1}^{-1} \cdot \tau_{n+1} \cdot \mathbf{F}_{n+1}^{-c} - \mathbf{F}_n^{-1} \cdot \tau_n \cdot \mathbf{F}_n^c] \cdot \mathbf{F}_{n+\alpha}^c + \frac{1}{\theta} \tau_{n+1} \\ &= \frac{2\eta}{\theta} \frac{1}{\Delta t} \mathbf{F}_{n+\alpha}^{-c} \cdot \frac{1}{2} [\mathbf{F}_{n+1}^c \cdot \mathbf{F}_{n+1} - \mathbf{F}_n^c \cdot \mathbf{F}_n] \cdot \mathbf{F}_{n+\alpha}^{-1} \end{aligned} \quad (79)$$

Though the above algorithm is incrementally objective for all $\alpha \in [0, 1]$, physically acceptable results are obtained only for $\alpha = \frac{1}{2}$. This is illustrated by the following example. Assume that the material is subjected to simple shear as depicted in Figure 2, that is

$$\mathbf{F}(t) = \begin{bmatrix} 1 & \gamma t & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (80)$$

Let $\{\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z\}$ denote a Cartesian vector base. Figure 3 shows $\tau_{yy} = \tau : \mathbf{e}_y \mathbf{e}_y$ at steady state shearing with a shear rate $\gamma = 0.1$ after one time step of $\Delta t = 1$, as a function of α , with parameters $\eta = 1^{10}$, $\theta = 10^{10}$. For this parameter setting, the UCM model virtually reduces to that of a purely elastic neo-Hookean medium. In that case $\tau : \mathbf{e}_y \mathbf{e}_y$ must be equal to 0. This is only the case for $\alpha = \frac{1}{2}$. Hence this choice not only gives second order accuracy, but also makes physical sense.

Figure 2. 2-D simple shear in x-y plane

Figure 3. Effect of α on τ_{yy}

PROBLEM DEFINITION

Presuming the extra stress tensor τ to be known at t_n , the algorithms indicated by propositions 1 and 2 are used to calculate τ_{n+1} .

The incompressibility constraint is written as

$$\det(\mathbf{F}) = 1 \quad (81)$$

Remark. The state at $t = t_n$ is chosen as the reference configuration of time interval S_n . This approach is referred to as the *Updated-Lagrangian* method. This implies that $\mathbf{F}_n = \mathbf{I}$.

The semi-discretized problem on S_n may be written as

Problem 1 ($\mathbf{P}_n$). Let the motion during S_n satisfy

$$\boldsymbol{\varphi}_{n+\alpha} = (1 - \alpha)\boldsymbol{\varphi}_n + \alpha\boldsymbol{\varphi}_{n+1}, \quad \alpha = \frac{t - t_n}{\Delta t} \in [0, 1], t \in S_n \quad (82)$$

and assume $\boldsymbol{\tau}_n$ to be known; then, given a body force $\mathbf{f}(\boldsymbol{\varphi}_{n+1}, t_{n+1}): \Omega \mapsto \mathbb{R}^n$, a boundary load $\mathbf{p}(\boldsymbol{\varphi}_{n+1}, t_{n+1}): \Gamma_p \mapsto \mathbb{R}^n$ and a prescribed motion $\boldsymbol{\varphi}^0: \Gamma_u \mapsto \mathbb{R}^n$, find the motion $\boldsymbol{\varphi}(\mathbf{x}_0, t_{n+1}): \Omega_0 \mapsto \mathbb{R}^n$ and the pressure field $p(\mathbf{x}, t_{n+1}): \Omega \mapsto \mathbb{R}$ such that

$$\nabla \cdot (-p_{n+1} \mathbf{I} + \boldsymbol{\tau}_{n+1}) + \mathbf{f}_{n+1} = \mathbf{0} \quad \text{in } \Omega \quad (83)$$

$$\det(\mathbf{F}_{n+1}) - 1 = 0 \quad \text{in } \Omega \quad (84)$$

$$\boldsymbol{\sigma}_{n+1} = \boldsymbol{\sigma}_{n+1}^c, \quad \boldsymbol{\sigma}_{n+1} = -p_{n+1} \mathbf{I} + \boldsymbol{\tau}_{n+1} \quad (85)$$

$$\boldsymbol{\varphi}_{n+1} = \boldsymbol{\varphi}_{n+1}^0 \quad \text{on } \Gamma_u \quad (86)$$

$$\boldsymbol{\sigma}_{n+1} \cdot \mathbf{n}_{n+1} = \mathbf{p}_{n+1} \quad \text{on } \Gamma_p \quad (87)$$

while the extra stress tensor satisfies

$$\begin{aligned} & \frac{1}{\Delta t} \mathbf{F}_{n+\alpha} \cdot [\mathbf{F}_{n+1}^{-1} \cdot \boldsymbol{\tau}_{n+1} \cdot \mathbf{F}_{n+1}^{-c} - \boldsymbol{\tau}_n] \cdot \mathbf{F}_{n+\alpha}^c + \frac{1}{\theta} \boldsymbol{\tau}_{n+1} \\ &= \frac{2\eta}{\theta} \frac{1}{\Delta t} \mathbf{F}_{n+\alpha}^{-c} \cdot \frac{1}{2} [\mathbf{F}_{n+1}^c \cdot \mathbf{F}_{n+1} - \mathbf{I}] \cdot \mathbf{F}_{n+\alpha}^{-1} \end{aligned} \quad (88)$$

WEAK FORMULATIONS

First the Arbitrary-Lagrange-Euler (ALE) formulation is discussed. Thereafter a simplified form (U-ALE) of the ALE formulation is explained.

ALE

In a Lagrangian formulation, all parameters are considered as functions of the material co-ordinates (for instance the reference co-ordinates $\mathbf{x}_0$ of each material point), while in the Eulerian formulation all parameters are taken as a function of the current spatial co-ordinates, i.e. $\mathbf{x}$. In an ALE formulation the description is with respect to the grid co-ordinates, i.e. $\mathbf{x}_g$. The motion of the grid points may be chosen independent of the motion of the material points.

The CRS domain Ω_g is always assumed to span the same space in $\mathbb{R}^3$ as the MRS domain Ω , hence their boundaries must coincide, e.g. $\Gamma_g = \Gamma$. The boundary Γ is split in two disjoint parts Γ_u and Γ_p . On Γ_u essential boundary conditions are given, while natural boundary conditions are prescribed along Γ_p .

Define the motion space $\mathcal{X}$ as

$$\mathcal{X} = \{\boldsymbol{\varphi} | \boldsymbol{\varphi}(\mathbf{x}_0) \in [\mathcal{C}^0(\Omega_0)]^3, \boldsymbol{\varphi} = \boldsymbol{\varphi}^0 \quad \text{on } \Gamma_u\} \quad (89)$$

where $\mathcal{C}^0(\Omega_0)$ denotes the space of continuous functions on Ω_0 . Notice that the motion $\boldsymbol{\varphi}$ describes the motion of *material* points. For non-linear problems it is rather difficult to precisely specify the integrability requirements. This is beyond the scope of the present paper.

The space of weight functions $\mathcal{W}$ is defined as a function of the grid positions by

$$\mathcal{W} = \{\mathbf{w} | \mathbf{w}(\mathbf{x}_g) \in [\mathcal{C}^0(\Omega_g)]^3, \mathbf{w} = \mathbf{0} \quad \text{on } \Gamma_u\} \quad (90)$$

while the space of pressure trial functions (and pressure weight functions) is defined as

$$\mathcal{Q} = \{q \mid q(\mathbf{x}_g) \in [\mathcal{C}^{-1}(\Omega_g)]^3\} \quad (91)$$

The ALE formulation is described by a set of two problems that yields a *decoupled* mixed formulation

Problem 2 (ALE_n). Let the motion $\boldsymbol{\varphi}$ during S_n satisfy

$$\boldsymbol{\varphi}_{n+\alpha} = (1 - \alpha)\boldsymbol{\varphi}_n + \alpha\boldsymbol{\varphi}_{n+1}, \quad \alpha = \frac{t - t_n}{\Delta t} \in [0, 1], \quad t \in S_n \quad (92)$$

let the motion $\boldsymbol{\varphi}_g$ either be known or be coupled to the motion of the material points (e.g. $\boldsymbol{\varphi}_g = \boldsymbol{\varphi}_g(\boldsymbol{\varphi})$), and assume $\boldsymbol{\tau}_n$ to be known, then, given $\mathbf{f}, \mathbf{p}$ and $\boldsymbol{\varphi}^0$ as before, find $(\boldsymbol{\varphi}_{n+1}, p_{n+1}) \in \mathcal{X} \times \mathcal{Q}$ such that

$$A(\mathbf{w}, p_{n+1}, \boldsymbol{\varphi}_{n+1}) = L(\mathbf{w}, \boldsymbol{\varphi}_{n+1}) \quad \forall \mathbf{w} \in \mathcal{W} \quad (93)$$

$$B(q, \boldsymbol{\varphi}_{n+1}) = 0 \quad \forall q \in \mathcal{Q} \quad (94)$$

with

$$A(\mathbf{w}, p_{n+1}, \boldsymbol{\varphi}_{n+1}) = \int_{\Omega_g} (\nabla \mathbf{w})^c : (-p_{n+1} \mathbf{I} + \boldsymbol{\tau}_{n+1}) d\Omega \quad (95)$$

$$L(\mathbf{w}, \boldsymbol{\varphi}_{n+1}) = \int_{\Omega_g} \mathbf{w} \cdot \mathbf{f}_{n+1} d\Omega + \int_{\Gamma_p} \mathbf{w} \cdot \mathbf{p}_{n+1} d\Omega \quad (96)$$

$$B(q, \boldsymbol{\varphi}_{n+1}) = \int_{\Omega_g} q(\det(\mathbf{F}_{n+1}) - 1) d\Omega \quad (97)$$

while the extra stress tensor $\boldsymbol{\tau}_{n+1}(\mathbf{x}_g)$ is found by solving problem ADV_n, i.e. Problem 3.

The extra stress tensor is found by solving the following advection problem on S_n :

$$\frac{\delta \boldsymbol{\tau}}{\delta t} = \dot{\boldsymbol{\tau}} + (\mathbf{v}_g - \mathbf{v}) \cdot \nabla \boldsymbol{\tau} \quad (98)$$

On S_n , the material rate is approximated by

$$\dot{\boldsymbol{\tau}} = \frac{\boldsymbol{\tau}_{n+1} - \boldsymbol{\tau}_n}{\Delta t} \quad (99)$$

where $\boldsymbol{\tau}_{n+1}$ is obtained from equation (88). For notational convenience, the abbreviation $\mathbf{M} = 1/\Delta t(\boldsymbol{\tau}_{n+1} - \boldsymbol{\tau}_n)$ is introduced. It should be kept in mind that equation (88) holds for a *material point*. Further, $\mathbf{v}_g$ and $\mathbf{v}$ are approximated by

$$\mathbf{v}_g = \frac{\Delta_g \mathbf{x}_g}{\Delta t} \quad (100)$$

and

$$\mathbf{v} = \frac{\Delta_m \mathbf{x}}{\Delta t} \quad (101)$$

respectively.

Introduce the operator

$$\underline{\mathcal{L}} = \left[\frac{\delta}{\delta t} - \left(\frac{\Delta_g \mathbf{x}_g}{\Delta t} - \frac{\Delta_m \mathbf{x}_m}{\Delta t} \right) \cdot \mathbf{e}_i \frac{\partial}{\partial x_i} \right] \underline{I}_6 \quad (102)$$

where $\underline{I}_6$ is the 6×6 unit matrix, and the columns

$$\underline{\tau}^T = [\tau_{11} \ \tau_{12} \ \tau_{22} \ \tau_{13} \ \tau_{23} \ \tau_{33}] \quad (103)$$

and

$$\underline{m}^T = [M_{11} \ M_{12} \ M_{22} \ M_{13} \ M_{23} \ M_{33}] \quad (104)$$

Then, the advection problem can be written as

$$\underline{\mathcal{L}}\underline{\tau} = \underline{m} \quad (105)$$

The advection step is numerically solved by application of a space-time finite element method as described in Shakib¹⁶ and Hughes *et al.*¹¹ and applied in 2-D viscoelastic flow by Baaijens.¹

In a space-time finite element method, the domain $\Omega \times S$ is divided into *space-time slabs*, defined by

$$Q_n = \Omega \times S_n \quad (106)$$

with boundary

$$P_n = \Gamma \times S_n \quad (107)$$

A space-time element can be defined as

$$Q_n^e = \Omega^e \times S_n \quad e = 1, \dots, n_{el} \quad (108)$$

Now, define the space of stress trial solutions as

$$S_n = \{\underline{\tau} | \underline{\tau}(\mathbf{x}, t) \in [\mathcal{C}^0(Q_n)]^6, \quad \underline{\tau} = \underline{\tau}^0 \text{ on } P_{nt}\} \quad (109)$$

and the space of stress weighting functions as

$$\mathcal{V}_n = \{\underline{v} | \underline{v}(\mathbf{x}, t) \in [\mathcal{C}^0(Q_n)]^6, \underline{v} = 0 \text{ on } P_{nt}\} \quad (110)$$

Application of the TD/GLS methodology to the advection problem yields the following weak form:

Problem 3 (ADV_n). Given $\Delta_m \mathbf{x}$, $\Delta_g \mathbf{x}_g$ and $\tau(\mathbf{x}, t_n)$, find $\underline{\tau}(\mathbf{x}, t) \in S_n$ such that for all $\underline{v}(\mathbf{x}, t) \in \mathcal{V}_n$

$$\begin{aligned} & \underbrace{\int_{Q_n} \underline{v}^T \underline{\mathcal{L}} \underline{\tau} dQ_n}_{\text{Galerkin}} + \sum_{e=1}^{n_{el}} \underbrace{\int_{Q_n^e} (\underline{\mathcal{L}} \underline{v})^T \underline{\lambda} \underline{\mathcal{L}} \underline{\tau} dQ_n}_{\text{GLS}} \\ & + \sum_{e=1}^{n_{el}} \underbrace{\int_{Q_n^e} \lambda_D (\underline{\nabla}_\xi \underline{v})^T (\underline{\nabla}_\xi \underline{\tau}) dQ_n}_{\text{Discontinuity capturing}} \\ & + \underbrace{\int_{\Omega} [v(t_n^+)^T (\underline{\tau}(t_n^+) - \underline{\tau}(t_n^-))] d\Omega}_{\text{Jump condition}} \\ & = \int_{Q_n} \underline{v}^T \underline{m} dQ_n + \sum_{e=1}^{n_{el}} \int_{Q_n^e} (\underline{\mathcal{L}} \underline{v})^T \underline{\lambda} \underline{m} dQ_n \end{aligned} \quad (111)$$

Let $\square$ denote a quadruple-unit cube with local co-ordinates ξ_1, ξ_2, ξ_3 and ξ_t , such that

$\mathbf{x}(\xi): \square \mapsto Q_n^e = \Omega^e \times S_n$. Then, inspired by Shakib,¹⁶

$$\underline{\lambda} = \lambda \underline{I}, \quad \lambda = \frac{\Delta t}{2} + \left[\frac{\partial \xi_i}{\partial x_j} \frac{\partial \xi_i}{\partial x_k} v_j v_k \right]^{-1/2} \quad i, j, k = 1, 3 \quad (112)$$

$$\lambda_D = 2 \frac{\|\underline{\mathcal{L}}\underline{\tau} - \underline{m}\|_\lambda^2}{\|\underline{\nabla}_\xi \underline{\tau}\|^2} \quad (113)$$

$$\underline{\nabla}_\xi^T = \left[\underline{I} \frac{\partial}{\partial \xi_1} \underline{I} \frac{\partial}{\partial \xi_1} \underline{I} \frac{\partial}{\partial \xi_2} \underline{I} \frac{\partial}{\partial \xi_3} \underline{I} \right] \quad (114)$$

Remark. The additional advection induced by the mesh movement in the ALE formulation may upset the objective integration scheme somewhat. Therefore, it is essential to apply a high order accurate scheme to integrate equation (98). The TD/GLS method is an accurate scheme, particularly if a linear in time approximation is used.

U-ALE

In a simplified ALE formulation (U-ALE) the CRS is *fixed* to the MRS during each *time step*. In that case there is no need to apply a mixed formulation to obtain the stresses. Hence, the stress field and displacement field are obtained directly from problem $\mathbf{ALE}_n$ without the solution of the advection step. The stress field is calculated directly from equation (88).

However, at the end of each time step the CRS is adjusted according to some specified method. The adjusted CRS is taken as the reference configuration for the next time step. In analogy with the updated Lagrangian methods, this approach is called the *Updated-ALE* (hence the abbreviation U-ALE) approach. To determine the stress field in the new, adjusted, state, the advection problem $\mathbf{ADV}_n$ is solved.

The advantages of this modification are as follows. Because of the decoupling employed in the mixed approach of the ALE formulation, the ultimate quadratic convergence of the Newton–Raphson procedure used to solve problem $\mathbf{ALE}_n$ is lost, as is demonstrated later. Further, the solution of the advection problem $\mathbf{ADV}_n$ is rather time consuming, and it must be obtained every iteration. In the U-ALE approach, quadratic convergence during the Lagrangian step is maintained, and the advection problem needs to be solved only once every time step. Both factors lead to a substantial saving in computation time.

The disadvantage of the U-ALE approach is that the advected stress that serves as an initial condition of the next time step does not satisfy the equilibrium equation. However, it will be shown that the differences between the ALE and U-ALE formulations are marginal. Therefore, virtually all calculations are performed with the U-ALE approach.

FINITE ELEMENT APPROXIMATION

Let $\hat{\Omega}$ be any known, convenient, configuration and let $\mathbf{z}_g$ denote the position of a particle in this configuration, e.g. $\mathbf{z}_g \in \hat{\Omega}$.

Finite dimensional approximations of $\mathcal{X}$, $\mathcal{W}$ and $\mathcal{Q}$, respectively, are given by¹⁰

$$\mathcal{X}^h = \{ \boldsymbol{\varphi}^h | \boldsymbol{\varphi}^h \in [\mathcal{C}^0(\Omega_{g0})]^3, \boldsymbol{\varphi}^h|_{\Omega^e} = \tilde{N}^T(\mathbf{z}_{g0})\boldsymbol{\varphi}(t), \boldsymbol{\varphi}^h = \boldsymbol{\varphi}^0 \text{ on } \Gamma_u \} \quad (115)$$

$$\mathcal{W}^h = \{ \mathbf{w}^h | \mathbf{w}^h \in [\mathcal{C}^0(\Omega_g)]^3, \mathbf{w}^h|_{\Omega^e} = \tilde{N}^T(\mathbf{z}_g)\mathbf{w}(t), \mathbf{w}^h = \mathbf{0} \text{ on } \Gamma_u \} \quad (116)$$

$$\mathcal{Q}^h = \{ q^h | q^h \in L_2(\Omega_g), q^h|_{\Omega^e} = \tilde{M}^T(\mathbf{z}_g)q(t) \} \quad (117)$$

where N and M contain shape functions.

The trial solutions $\mathcal{S}_n$ and weighting functions $\mathcal{V}_n$ are approximated by k th-order interpolation polynomials, $\mathcal{P}_k(Q_n^e)$. These are chosen $\mathcal{C}^0$ continuous within each space-time slab, but are discontinuous across the interfaces of each time slab. Hence

$$\mathcal{S}_n^h = \{\tau | \tau \in [\mathcal{C}^0(Q_n)]^6, \tau|_{Q_n^e} \in [\mathcal{P}_k(Q_n^e)]^6, \tau = \tau^0 \text{ on } P_{n\tau}\} \quad (118)$$

and

$$\mathcal{V}_n^h = \{v | v \in [\mathcal{C}^0(Q_n)]^6, v|_{Q_n^e} \in [\mathcal{P}_k(Q_n^e)]^6, v = 0 \text{ on } P_{n\tau}\} \quad (119)$$

NEWTON-RAPHSON ITERATION PROCESS

Problem ALE_n is solved iteratively with the Newton-Raphson iteration process.

Define the directional derivative of a functional $A(\mathbf{w}, p, \boldsymbol{\varphi})$ in the direction $\delta\boldsymbol{\varphi}$ with respect to the third variable as

$$\delta_{\boldsymbol{\varphi}} A(\mathbf{w}, p, \boldsymbol{\varphi}; \delta\boldsymbol{\varphi}) = \lim_{\theta \rightarrow 0} \frac{A(\mathbf{w}, p, \boldsymbol{\varphi} + \theta\delta\boldsymbol{\varphi}) - A(\mathbf{w}, p, \boldsymbol{\varphi})}{\theta} \quad (120)$$

Likewise, define

$$\delta_p A(\mathbf{w}, p, \boldsymbol{\varphi}; \delta p) = \lim_{\theta \rightarrow 0} \frac{A(\mathbf{w}, p + \theta\delta p, \boldsymbol{\varphi}) - A(\mathbf{w}, p, \boldsymbol{\varphi})}{\theta} \quad (121)$$

Analogously, the directional derivative of a tensor $\mathbf{A}(\boldsymbol{\varphi})$ in the direction $\delta\boldsymbol{\varphi}$ is defined as

$$\delta\mathbf{A}(\boldsymbol{\varphi}; \delta\boldsymbol{\varphi}) = \lim_{\theta \rightarrow 0} \frac{\mathbf{A}(\boldsymbol{\varphi} + \theta\delta\boldsymbol{\varphi}) - \mathbf{A}(\boldsymbol{\varphi})}{\theta} \quad (122)$$

Now, let $\mathbf{y}$ be an estimate of the motion $\boldsymbol{\varphi}$, $\delta\boldsymbol{\varphi}$ the error in the estimate $\mathbf{y}$, and let r be an estimate of the pressure p , with δp the error in the estimate:

$$\boldsymbol{\varphi} = \mathbf{y} + \delta\boldsymbol{\varphi} \quad (123)$$

$$p = r + \delta p \quad (124)$$

The non-linear forms $A(\cdot, \cdot, \cdot)$, $B(\cdot, \cdot)$ and $L(\cdot, \cdot)$ may be written as

$$A(\mathbf{w}, r, \mathbf{y}) + \delta_{\boldsymbol{\varphi}} A(\mathbf{w}, r, \mathbf{y}; \delta\boldsymbol{\varphi}) + \delta_p A(\mathbf{w}, r, \mathbf{y}; \delta p) + \cdots \quad (125)$$

$$B(q, \mathbf{y}) + \delta_{\boldsymbol{\varphi}} B(q, \mathbf{y}; \delta\boldsymbol{\varphi}) + \cdots \quad (126)$$

$$L(\mathbf{w}, \mathbf{y}) + \delta_{\boldsymbol{\varphi}} L(\mathbf{w}, \mathbf{y}; \delta\boldsymbol{\varphi}) + \cdots \quad (127)$$

Introduce the following 'error' spaces:

$$\delta\mathcal{X}_0 = \{\delta\boldsymbol{\varphi} | \delta\boldsymbol{\varphi} \in [\mathcal{C}^0(\Omega_g)]^3, \delta\boldsymbol{\varphi} = \mathbf{0} \text{ on } \Gamma_u\} \quad (128)$$

$$\delta\mathcal{X}_{n+1} = \{\delta\boldsymbol{\varphi} | \delta\boldsymbol{\varphi} \in [\mathcal{C}^0(\Omega_g)]^3, \delta\boldsymbol{\varphi} = \boldsymbol{\varphi}^0(\mathbf{x}_0, t_{n+1}) - \boldsymbol{\varphi}^0(\mathbf{x}_0, t_n) \text{ on } \Gamma_u\} \quad (129)$$

With these linearizations the Newton-Raphson iteration process can be outlined as follows.

1. Initialization:

$$i = 1, \quad \mathbf{y} = \mathbf{y}_n \quad (130)$$

2. If $i = 1$ then $\delta\mathcal{X}_a = \delta\mathcal{X}_{n+1}$ else $\delta\mathcal{X}_a = \delta\mathcal{X}_0$. Find $(\delta^i \mathbf{y}, \delta^i p) \in \delta\mathcal{X}_a \times \mathcal{Q}$ such that

$$\delta_{\boldsymbol{\varphi}} A(\mathbf{w}, r^i, \mathbf{y}^i; \delta^i \mathbf{y}) + \delta_p A(\mathbf{w}, r^i, \mathbf{y}^i; \delta^i p) - \delta_{\boldsymbol{\varphi}} L(\mathbf{w}, \mathbf{y}^i; \delta^i \mathbf{y})$$

$$= -A(\mathbf{w}, r^i, \mathbf{y}^i) + L(\mathbf{w}, \mathbf{y}^i) \quad \forall \mathbf{w} \in \mathcal{W} \quad (131)$$

$$\delta_\varphi B(q, \mathbf{y}^i; \delta^i \mathbf{y}) = -B(q, \mathbf{y}^i) \quad \forall q \in \mathcal{Q} \quad (132)$$

3. Update $i, \mathbf{y}^i$ and r :

$$i \leftarrow i + 1, \quad \mathbf{y}^i \leftarrow \mathbf{y}^i + \delta^i \mathbf{y}, \quad r^i \leftarrow r^i + \delta^i p \quad (133)$$

4. Repeat from step 2 until convergence.

Clearly, the main task to be performed in a Newton–Raphson iteration process is the evaluation of $\delta_\varphi A$, $\delta_p A$, $\delta_\varphi B$ and $\delta_\varphi L$.

Calculation of $\delta_\varphi A$ and $\delta_p A$

Using $\nabla = \mathbf{F}_g^{-c} \cdot \nabla_0$, the functional $A(\cdot, \cdot, \cdot)$ is rewritten as

$$A(\mathbf{w}, p, \boldsymbol{\varphi}) = \int_{\Omega_g} (\nabla \mathbf{w})^c : (-p\mathbf{I} + \boldsymbol{\tau}) \, d\Omega \quad (134)$$

$$= \int_{\Omega_g} (\nabla_0 \mathbf{w})^c : \mathbf{F}_g^{-1} \cdot (-p\mathbf{I} + \boldsymbol{\tau}) \, d\Omega \quad (135)$$

The above transformation implies that integration takes place over the CRS domain. Therefore, the following relation must be obeyed in evaluating $\boldsymbol{\tau}$:

$$\begin{aligned} \boldsymbol{\tau}(\mathbf{x}_g) &= \boldsymbol{\tau}_0 + \Delta_g \boldsymbol{\tau} \\ &= \boldsymbol{\tau}_0 + \Delta_m \boldsymbol{\tau} + (\Delta_g \mathbf{x}_g - \Delta_m \mathbf{x}) \cdot \nabla \boldsymbol{\tau} \end{aligned} \quad (136)$$

Application of the definition of $\delta_\varphi A$ yields

$$\delta_\varphi A = \int_{\Omega_g} (\nabla_0 \mathbf{w})^c : [\delta(\mathbf{F}_g^{-1}) \cdot (-p\mathbf{I} + \boldsymbol{\tau}) + \mathbf{F}_g^{-1} \cdot \delta \boldsymbol{\tau}] \, d\Omega \quad (137)$$

and, likewise it follows that

$$\delta_p A = \int_{\Omega_g} (\nabla_0 \mathbf{w})^c : \mathbf{F}_g^{-1} \cdot (-\delta p \mathbf{I}) \, d\Omega \quad (138)$$

So, $\delta(\mathbf{F}_g^{-1})$ and $\delta \boldsymbol{\tau}$ remain to be calculated.

Calculation of linearized deformation tensor. Introduce the abbreviations

$$\mathbf{L}_\delta \stackrel{\text{def}}{=} (\nabla_0 \delta \boldsymbol{\varphi})^c \cdot \mathbf{F}^{-1} \quad (139)$$

$$= (\nabla \delta \boldsymbol{\varphi})^c \quad (140)$$

and

$$\mathbf{L}_{\delta g} \stackrel{\text{def}}{=} (\nabla_0 \delta \boldsymbol{\varphi}_g)^c \cdot \mathbf{F}_g^{-1} \quad (141)$$

$$= (\nabla \delta \boldsymbol{\varphi}_g)^c \quad (142)$$

Then,

$$\delta(\mathbf{F}^{-1}) = -\mathbf{F}^{-1} \cdot \mathbf{L}_\delta \quad (143)$$

and

$$\delta(\mathbf{F}_g^{-1}) = -\mathbf{F}_g^{-1} \cdot \mathbf{L}_{\delta g} \quad (144)$$

Clearly, equation (144) is relevant only if the motion of the gridpoints is not prescribed entirely. If it is not prescribed then, as we have stated before, it is coupled to the motion of the material points. Hence $\delta\boldsymbol{\varphi}_g$ could be expressed in $\delta\boldsymbol{\varphi}$. However, the above expression is used in the subsequent development, and the coupling is addressed later.

Calculation of linearized extra stress tensor. In the process of linearizing the extra stress tensor it is assumed that a fully implicit scheme is chosen, e.g. $\alpha = 1$, irrespective of what value for α is actually chosen in calculating $\boldsymbol{\tau}_{n+1}$. The consequence of this may be a lower convergence speed.

Define

$$\hat{\boldsymbol{\tau}} = \frac{\theta}{\theta + \Delta t} \mathbf{F} \cdot \boldsymbol{\tau}_n \cdot \mathbf{F}^c \quad \text{and} \quad \tilde{G} = \frac{\eta}{\theta + \Delta t}.$$

A direct application of equation (122) to the definition of $\boldsymbol{\tau}$ gives

$$\delta\boldsymbol{\tau} = \mathbf{L}_\delta \cdot \hat{\boldsymbol{\tau}} + \hat{\boldsymbol{\tau}} \cdot \mathbf{L}_\delta^c + \tilde{G}[\mathbf{L}_\delta^c \cdot \mathbf{B} + \mathbf{B} \cdot \mathbf{L}_\delta] + (\delta\boldsymbol{\varphi}_g - \delta\boldsymbol{\varphi}) \cdot \nabla \boldsymbol{\tau} \quad (145)$$

with $\mathbf{B} = \mathbf{F}^{-c} \cdot \mathbf{F}^{-1}$. Using equation (143) and (145) it follows that

$$\begin{aligned} \delta_\varphi A = \int_{\Omega_g} (\nabla \mathbf{w})^c : [& -\mathbf{L}_{\delta g} \cdot (-p\mathbf{I} + \boldsymbol{\tau}) \\ & + \mathbf{L}_\delta \cdot \hat{\boldsymbol{\tau}} + \hat{\boldsymbol{\tau}} \cdot \mathbf{L}_\delta^c + \tilde{G}(\mathbf{L}_\delta^c \cdot \mathbf{B} + \mathbf{B} \cdot \mathbf{L}_\delta) \\ & + (\delta\boldsymbol{\varphi}_g - \delta\boldsymbol{\varphi}) \cdot \nabla \boldsymbol{\tau}] d\Omega \end{aligned} \quad (146)$$

Calculation of $\delta_\varphi B$

The form $\delta_\varphi B$ is calculated as

$$\delta_\varphi B(q, \boldsymbol{\varphi}; \delta\boldsymbol{\varphi}) = \int_{\Omega_g} q \delta(\det(\mathbf{F})) d\Omega \quad (147)$$

$$= \int_{\Omega_g} q \det(\mathbf{F}) \operatorname{tr}(\mathbf{L}_\delta) d\Omega \quad (148)$$

It is useful to rewrite the linearized weak form of the incompressibility constraint

$$B(q, \boldsymbol{\varphi}) + \delta_\varphi B(q, \boldsymbol{\varphi}; \delta\boldsymbol{\varphi}) = \int_{\Omega_g} q(\det(\mathbf{F}) - 1) d\Omega + \int_{\Omega_g} q \det(\mathbf{F}) \operatorname{tr}(\nabla \delta\boldsymbol{\varphi}) d\Omega = 0 \quad (149)$$

as

$$\underbrace{- \int_{\Omega_g} q \frac{(\det(\mathbf{F}) - 1)}{\det(\mathbf{F})} d\Omega}_{\tilde{B}} - \underbrace{\int_{\Omega_g} q \operatorname{tr}(\nabla \delta\boldsymbol{\varphi}) d\Omega}_{\delta_\varphi \tilde{B}} = 0 \quad (150)$$

Formally, this is achieved by replacing the weighting function q in equation (149) with a new weighting function $\hat{q} = q/\det(\mathbf{F})$.

Calculation of $\delta_\phi L$

In most common non-linear finite element codes the form $\delta_\phi L$ is neglected, because the contribution of this term to the coefficient matrix is, in general, small compared to the contributions of $\delta_\phi A$ and $\delta_p A$. At worst, this leads to slightly lower speed of convergence of the Newton–Raphson process. In the present work, too, the contribution of $\delta_\phi L$ is neglected.

IMPLEMENTATION ASPECTS

Let the motion space of the CRS points be given by

$$\mathcal{X}_g = \{\boldsymbol{\varphi}_g | \boldsymbol{\varphi}_g(\mathbf{x}_{0g}) \in [\mathcal{C}^0(\Omega_{g0})]^3\} \quad (151)$$

This space is discretized in the same way as $\mathcal{X}$, e.g.

$$\mathcal{X}_g^h = \{\boldsymbol{\varphi}_g^h | \boldsymbol{\varphi}_g^h \in [\mathcal{C}^0(\Omega_{g0})]^3, \boldsymbol{\varphi}^h|_{\Omega^e} = \mathbf{N}^T(\mathbf{z}_{g0})\boldsymbol{\varphi}_g(t)\} \quad (152)$$

As was indicated before, the motion of the grid is coupled to the motion of the material points. This is achieved by coupling the motion of the nodal points of the CRS, $\boldsymbol{\varphi}_{ga}$, to the motion of the nodal points of the MRS, $\boldsymbol{\varphi}$:

$$\boldsymbol{\varphi}_{ga}(t) = \boldsymbol{\Psi}(\boldsymbol{\varphi}_a(t)), \quad t = S_n \quad (153)$$

where $\boldsymbol{\varphi}_a$ is chosen such that

$$\mathbf{x}_{ga}(t_n) = \mathbf{x}_a(t_n) \quad (154)$$

In all cases presented later on, this relation is chosen as

$$\boldsymbol{\varphi}_{ga} = (\mathbf{I} - \mathbf{d}\mathbf{d}): \boldsymbol{\varphi}_a \quad (155)$$

with $\mathbf{d}$ some specified unit direction.

The demand that the boundary of the grid domain coincides with the boundary of the material domain can be achieved only at the nodal points of the grid. Yet, equation (155) would violate this constraint. Therefore, nodal points of the CRS boundary are projected onto the material boundary after each iteration along the unit outward normal subject to relation (155). Hence, if $\mathbf{n}$ is the unit outward normal of Γ , the projection direction is $\mathbf{n} - \mathbf{n} \cdot \mathbf{d}\mathbf{d}$.

CONTACT CONDITIONS

In the U-ALE formulation a contact algorithm is implemented as well. Let Ω_R denote a rigid body with boundary Γ_R that may not be penetrated. The function $g(\mathbf{x})$ is defined such that (see Baaijens *et al.*³)

$$g(\mathbf{x}) < 0 \quad \text{if } \mathbf{x} \ni \Omega_R \quad (156)$$

$$g(\mathbf{x}) = 0 \quad \text{if } \mathbf{x} \in \Gamma_R \quad (157)$$

$$g(\mathbf{x}) > 0 \quad \text{if } \mathbf{x} \in \Omega_R \quad (158)$$

Further, the contact pressure $\sigma_n = \boldsymbol{\sigma} : \mathbf{n}\mathbf{n}$ must be non-positive, and it may only be less than zero if $g = 0$. Hence, the complete contact conditions are

$$g(\mathbf{x}) \leq 0, \quad \sigma_n g = 0, \quad \sigma_n \leq 0 \quad \forall \mathbf{x} \in \Gamma_C \quad (159)$$

where Γ_C denotes the potential contact boundary of Ω . Friction is modelled with the following

regularized Coulomb friction law:

$$\sigma_t = -\mu\sigma_n \tanh\left(\frac{\mathbf{v}_s}{\varepsilon}\right) \frac{\mathbf{v}_s}{\|\mathbf{v}_s\|} \quad (160)$$

where $\sigma_t = \boldsymbol{\sigma} \cdot \mathbf{n} - \sigma_n \mathbf{n}$, $\mathbf{v}_s$ the sliding velocity and ε a regularization parameter. Clearly, more sophisticated models could be implemented as well, see Baaijens *et al.*²

The above contact conditions, including the friction equations, are enforced nodally with a Lagrange multiplier method; for more details see Baaijens *et al.*²

DISCRETIZATION

For the discretization of $\mathcal{X}^h$ the P_1 tri-linear brick element is used, while $\mathcal{Q}^h$ is discretized with a P_0 piecewise constant shape function. The components of the extra stress tensor τ as used in problem ALE_n are discretized in space with the P_1 tri-linear brick element, and with a discontinuous linear field in time. This is summarized in Table I.

EXAMPLES

First of all the performance of the ALE formulation is compared to the U-ALE formulation. Secondly, the U-ALE formulation is applied to the rolling contact problem of a viscoelastic material. Such a problem bears many resemblances with the capstan pinch-roller tape transport device in a video recorder. The major difference being the absence of a tape between the capstan and pinch-roller.

In all computations the discontinuity capturing coefficient λ_D is set to zero.

Example 1: Comparison of ALE with U-ALE

Consider the tapered bar indicated in Figure 4.

Table I. Discretization

Problem	Variable(s)	Space	Time
ALE _n	(φ, p)	$P_1 - P_0$	
ADV _n	τ	P_1	P_1

Figure 4. Tapered bar

The material is assumed to be neo-Hookean, e.g.

$$\boldsymbol{\tau} = c(\mathbf{B} - \mathbf{I}) \quad (161)$$

with $c = 1$. Neo-Hookean material behaviour is obtained as a limiting case of the UCM model if relaxation is disregarded.

The boundary conditions are as follows: in the xy -plane displacements in the z -direction are suppressed, in the yz -plane displacements in the x -direction are suppressed and in the xz -plane displacements in the y -direction are suppressed. The plane, initially at $z = 5$, is displaced in the positive z -direction by 0.25 at each increment. All other displacements at this plane are non-prescribed. Further, all nodes with a z -co-ordinate less than 3.01 are assumed to remain at their initial z position. Hence $\mathbf{d} = \mathbf{e}_z$ for these nodes. Figure 5 shows the deformed geometry after the fifth increment in case the ALE formulation is used. The results of the U-ALE formulation are

Figure 5. Deformed bar after the fifth increment

Figure 6. Cauchy stress in the z -direction for both the ALE and the U-ALE formulation

virtually identical. To compare the results of the ALE and the U-ALE formulation the σ_{zz} -component of the Cauchy stress tensor obtained with both formulations along the line $x = 0$, $y = 1.75$ is shown in Figure 6. The differences are small. The convergence behaviour, however, differs significantly. This is illustrated in Figure 7 where the energy norm is plotted as a function of the iteration number at increment 2. The slow convergence of the ALE formulation is attributed to the uncoupled stress calculation.

Example 2: Comparison of ALE with U-ALE in bending

Consider the bar depicted in Figure 8. Like in the previous example, neo-Hookean material behaviour is assumed with a constant $c = 1$.

Figure 7. Convergence comparison of the U-ALE and the ALE formulation

Figure 8. Rectangular bar

The boundary conditions are as follows: along the xz -plane all displacements are fixed, along the $y = 5$ plane the displacements in the y -direction are suppressed and along the $x = 2$ plane the displacements in the x -direction are suppressed. Finally, the displacements along the $z = 1.5$ plane are prescribed for all $y > 3$ in the z -direction. For the solution shown, the total z -displacement is -0.5 . Further, all grid points are assumed not to displace in the y -direction, hence $\mathbf{d} = \mathbf{e}_y$.

As a result the deformed geometry obtained with the U-ALE formulation is given in Figure 9. Secondly, the σ_{zz} solution along the line $x = 2$, $y \in [3.25, 5]$, $z = 1.5$ is compared in Figure 10.

The convergence behaviour is very similar to the previous example: U-ALE retained quadratic convergence, while ALE converged much slower.

Example 3: Rolling of viscoelastic strip

The U-ALE formulation is applied to the rolling of a viscoelastic strip with frictional contact conditions. Consider the strip as sketched in Figure 11.

The strip is modelled with the UCM model with parameters $\eta = \theta = 1$. The interpolation parameter α is set to 0.5.

As a boundary condition the displacements in the x - and z -directions are suppressed in the xy -plane. Further, a cylinder is indented having a radius of 2.3 and a point on the axis is

Figure 9. Deformed bar

Figure 10. Cauchy stress in the z -direction for the ALE and the U-ALE formulation in the bend bar

Figure 11. Computational domain

Table II. Parameter setting

Parameter	ω	μ	ε	Δt	θ	η	α
Equation		(160)	(160)	(46)	(42)	(42)	
Value	1	0.9	0.1	0.05	1	1	0.5

Figure 12. Deformed CRS after increment 10, U-ALE formulation

characterized by the following relation,

$$\mathbf{x}_{\text{axis}} = 3.5\mathbf{e}_y + 3.75\mathbf{e}_z + \lambda\mathbf{e}_x \quad (162)$$

with λ an arbitrary parameter used to identify each individual point on the axis. Clearly, a maximum indentation of 0.3 is achieved in this manner. The angular rotational speed ω of the cylinder along the x -axis is 1. The frictional coefficient is chosen to be 0.9, a characteristic value for rubbery materials in contact with steel. The penalty parameter ε in the frictional model is set to 0.1, while a time step of 0.05 is chosen. This parameter setting is summarized in Table II.

All grid nodes are assumed to remain at their original y position, hence $\mathbf{d} = \mathbf{e}_y$. Further, after the first time step, all interior grid nodes are assumed not to displace at all, so only the boundary nodes are adjusted to follow the material boundaries.

Material flows in and out of the computational domain. This implies that boundary conditions must be supplied at these in and out flow boundaries. Here, for simplicity, it is assumed that the stress state is zero at both the in and out flow boundary.

Figure 12 shows the deformed strip after 10 increments. The only relevant information in a plot like this is that it shows the contours of the computational domain. The actual material

Figure 13. Deformed CRS after increment 10, Lagrangian formulation

Figure 14. Displacement of the CRS along the line $x = 2$, $z = 1.75$

Figure 15. Cauchy stress in the z-direction

Figure 16. Effect of rotation angle, in degrees, on τ

displacements are not shown. As a comparison the deformed strip obtained with a pure Lagrangian computation is shown in Figure 13.

Figure 14 shows the displacement of the CRS points originally on the line $x = 2$, $z = 1.75$ at a number of times.

Finally, Figure 15 shows the σ_{zz} -distribution along that line at various times.

CONCLUSIONS

It is shown how the incremental objectivity requirements affect three dimensional viscoelastic flow computations. Further, a comparison is made between the Arbitrary-Lagrange-Euler (ALE) formulation and the so-called Updated-Arbitrary Lagrange-Euler (U-ALE) formulation. The latter is shown to be far more computationally efficient, while giving comparable results.

An important feature of the current implementation is the use of the Time-Discontinuous/Galerkin-Least-Squares (TD/GLS) formulation to handle the advective terms in the stress computation. This method has proven to be very accurate and is relatively simple to implement.

Finally, it is demonstrated that contact conditions can easily be incorporated in an U-ALE formulation.

APPENDIX

Aspects of objective numerical integration in a Eulerian formulation

Consider the Upper-Convected-Maxwell model (UCM)

$$\overset{\nabla}{\boldsymbol{\tau}} + \frac{1}{\theta} \boldsymbol{\tau} = \frac{2\eta}{\theta} \mathbf{D} \quad (163)$$

with

$$\overset{\nabla}{\boldsymbol{\tau}} = \frac{\partial \boldsymbol{\tau}}{\partial t} + \mathbf{v} \cdot \nabla \boldsymbol{\tau} - \mathbf{L} \cdot \boldsymbol{\tau} - \boldsymbol{\tau} \cdot \mathbf{L}^c \quad (164)$$

the Truesdell rate of $\boldsymbol{\tau}$.

In the Eulerian formulation commonly employed, $\mathbf{L}$, and hence $\mathbf{D}$, are given at each spatial location. Two ways to integrate equation (163) are investigated: first, a direct application of the midpoint integration scheme to equation (163), and, second, the algorithm proposed by Pinsky *et al.*¹⁴ and applied by van Hoogstraten *et al.*⁸

Remark. The results of the first method also hold for a Lagrangian formulation if in that case a direct integration of the constitutive equation is performed.

Consider a generic state transition $t_n \rightarrow t_{n+1}$, with $\Delta t = t_{n+1} - t_n$. A direct application of the generalized midpoint integration rule to equation (163) gives

$$\frac{\boldsymbol{\tau}_{n+1} - \boldsymbol{\tau}_n}{\Delta t} + \mathbf{v}_{n+\alpha} \cdot \nabla \boldsymbol{\tau}_{n+\alpha} - \mathbf{L}_{n+\alpha} \cdot \boldsymbol{\tau}_{n+\alpha} - \boldsymbol{\tau}_{n+\alpha} \cdot \mathbf{L}_{n+\alpha}^c = \frac{2\eta}{\theta} \mathbf{D}_{n+\alpha} \quad (165)$$

with

$$(\cdot)_{n+\alpha} = (1 - \alpha)(\cdot)_n + \alpha(\cdot)_{n+1} \quad (166)$$

The second algorithm is inspired by Theorem 1. For the Truesdell rate the invariant tensor associated with τ is given by

$$\bar{\tau} = \mathbf{F}^{-1} \cdot \tau \cdot \mathbf{F}^{-c} \quad (167)$$

while $\mathbf{F}$ satisfies

$$\dot{\mathbf{F}} = \mathbf{F} \cdot \mathbf{L} \quad (168)$$

Using equation (167), the UCM model is rewritten as

$$\dot{\bar{\tau}} + \frac{1}{\theta} \bar{\tau} = \frac{2\eta}{\theta} \bar{\mathbf{D}}, \quad \bar{\mathbf{D}} = \mathbf{F}^{-1} \cdot \mathbf{D} \cdot \mathbf{F}^{-c} \quad (169)$$

Implicit integration of this form yields

$$\frac{\bar{\tau}_{n+1} - \bar{\tau}_n}{\Delta t} + \mathbf{v} \cdot \nabla \tau_{n+1} + \frac{1}{\theta} \bar{\tau}_{n+1} = \frac{2\eta}{\theta} \bar{\mathbf{D}}_{n+1} \quad (170)$$

Based upon equation (168), neglecting convective terms and assuming $\mathbf{F}_n = \mathbf{I}$ (updated formula), Van Hoogstraten *et al.*⁸ proposed to approximate the deformation tensor by

$$\mathbf{F}_{n+1} = (\mathbf{I} - \alpha \Delta t \mathbf{L}_{n+1})^{-1} (\mathbf{I} + (1 - \alpha) \mathbf{L} \Delta t) \quad (171)$$

For $\alpha = 0.5$, this scheme produces a deformation tensor that is skew symmetric and has a unit determinant.

The two algorithms are compared for a sample problem, and non-objectivity of the algorithms is shown. Consider a homogeneous deformation of a body in 2-D. With respect to a Cartesian vector base $\{\mathbf{e}_1, \mathbf{e}_2\}$ the imposed rotation matrix is

$$\underline{\mathbf{R}} = \begin{bmatrix} \cos(\omega t) & -\sin(\omega t) \\ \sin(\omega t) & \cos(\omega t) \end{bmatrix} \quad (172)$$

hence, the velocity gradient matrix is given by

$$\underline{\mathbf{L}} = \begin{bmatrix} -\omega \sin(\omega t) & -\omega \cos(\omega t) \\ \omega \cos(\omega t) & -\omega \sin(\omega t) \end{bmatrix} \quad (173)$$

where ω is the speed of rotation. The extra stress matrix at $t = 0$ equals

$$\underline{\tau} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \quad (174)$$

In the elastic limit, the stress matrix at some time t should satisfy

$$\underline{\tau} = \underline{\mathbf{R}} \underline{\tau}_0 \underline{\mathbf{R}}^T \quad (175)$$

For a given state transition $t_n \rightarrow t_{n+1}$, the speed of rotation is selected such that the angle of rotation is varied.

Figure 16 shows the error in $\underline{\tau}$ as a function of the rotation in degrees if this rotation is imposed in one time step. The solid line is obtained when equations (170) and (171) are used, while the dashed line results with equation (165).

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