Numerical modelling of non-linear behaviour of soft biological materials

Satya N. Atluri and H. Murakawa
School of Engineering Science and Mechanics, Georgia Institute of Technology, Atlanta, Georgia, USA

Albert S. Kobayashi
Department of Mechanical Engineering, University of Washington, Seattle, Washington, USA
(Received 22 November 1978)

This paper deals with the formulation of rigorous numerical methods for the stress analysis, at finite strains, of soft biological materials that can be characterized as incompressible nonlinear elastic solids.

Introduction

Biological materials such as, for instance, the human skin, brain tissue, papillary muscles, and arteries are often characterized as nonlinear elastic materials. Various attempts at characterizing a strain-energy density function for such materials have been made.\textsuperscript{1-4} In normal physiological functioning, as well as in inadvertent circumstances such as injuries, these materials are subject to finite strains. For instance, as estimated in Danielson,\textsuperscript{1} the skin over the middle joint of a finger elongates about 20\% when the joint is bent. Likewise,\textsuperscript{5,6} the brain tissue may be subjected to strains of the order of 30\% in situations of head injury. This paper presents a summary of recent studies by the authors\textsuperscript{7-9} that deal with consistent and rigorous numerical methods for modelling such finite deformation problems, as above, for biological materials of the nonlinear elastic incompressible type.

Due to space limitations, the presentation is necessarily cursory; further details may be found elsewhere.\textsuperscript{7-9} The formulations presented are valid for an incompressible nonlinear elastic material with any general strain energy density function; specific forms of such strain energy functions\textsuperscript{1-4} can be implemented in a straightforward manner.

Theoretical formulation

For simplicity, the initial as well as the deformed configurations of the solid are referred to the same cartesian frame. We employ the following notation: \( _{\mu} \) under symbol denotes a tensor; \( _{\mu} \) under symbol denotes a vector; \( \phi \) and \( \psi \) are undeformed and deformed position vectors, respectively; \( \partial(\cdot) / \partial x_m; \nabla = \not_{m} (\partial / \partial x_m) \) is the gradient in undeformed metric; \( A \cdot B \) denotes product of two tensors such that \( (A \cdot B)_{ij} = A_{ik} B_{kj}; A \cdot B = \text{trace} (A^T \cdot B) = A_{ij} B_{ij}; u \cdot t = u_i t_i; \) and \( g = A^{-1} B \) such that \( a_i = A_{ik} b_k. \)

Then, the gradient of \( \psi \) is the tensor \( F \), such that:

\[
\nabla \psi = F \cdot d \psi \quad F = \nabla \psi \quad F_{ij} = \psi_{ij} \quad (1)
\]

In the above, the expression \( \nabla \psi \) does not mean the tensor product of \( \psi \) with \( \psi \), but is defined through equation (1).

The nonsingular \( F \) is considered to have the polar decomposition:

\[
F = g \cdot (L + h) \quad (2)
\]

where \( (L + h) \) is a symmetric positive-definite tensor, called the stretch tensor; \( L \) is the identity tensor; and \( g \) is an orthogonal rotation tensor such that \( g^T = g^{-1} \). The gradient of the displacement vector \( u \) is defined by:

\[
e = \nabla u; \quad e_{ij} = u_{i,j} \quad (3)
\]

The deformation tensor, \( G \), is defined by:

\[
G = F^T \cdot F = (h + L)^2 \quad (4)
\]

The three principal invariants of the deformation tensor are denoted by \( I_1, I_2 \) and \( I_3 \), respectively, such that:

\[
\frac{\partial f_1}{\partial G} = 1; \quad \frac{\partial f_2}{\partial G} = I_1 L - G; \quad \frac{\partial f_3}{\partial G} = I_3 G^{-1} \quad (5)
\]

If \( h_1, h_2 \) and \( h_3 \), respectively are the three principal invariants of the stretch tensor \( (L + h) \), it is further seen that:

\[
I_1 = h_1^2 - 2h_2; \quad I_2 = h_2^2 - 2h_3 h_1; \quad I_3 = h_3^2 \quad (6)
\]

The Green–Lagrange strain tensor is defined by:

\[
g = \frac{1}{2} (G - I) = \frac{1}{2} \left[ \nabla \psi + (\nabla \psi)^T + (\nabla \psi)^T \cdot (\nabla \psi) \right] \quad (7)
\]
As in references 7 and 8 we define the first and second Piola-Kirchhoff stresses \( \mathbf{\tau} \) and \( \mathbf{\Sigma} \), respectively, as measured per unit area in the initial configuration, in terms of the true (Euler) stress \( \mathbf{r} \) in the deformed configuration, through the relations:

\[
\mathbf{\tau} = \frac{1}{J} F^{-1} : \mathbf{\tau} = \frac{1}{J} F^{-1} : S : F^T
\]

(8)

or, inversely:

\[
\mathbf{\tau} = J(F^{-1}) : \mathbf{\tau} = J(F^{-1}) : \mathbf{\Sigma}(F^{-1})
\]

(9)

and

\[
\mathbf{\tau} = S : F^T
\]

(10)

where \( J \) is the determinant of the matrix \( \mathbf{y}_{mn} \).

Let the strain energy density per unit initial volume be \( W \). As is well known, the stress tensor in incompressible materials is determined by the strain-energy density function only to within an additive scalar, called the hydrostatic pressure denoted here by \( P \). The kinematic constraint of incompressibility, viz., \( I_3 = h_3 = 1.0 \) can be directly embedded in a modified definition of strain-energy density function, such that:

\[
W = W(g, P) = \mathbf{\hat{W}(g)} + \frac{P}{2}(I_3 - 1)
\]

(11)

or alternatively:

\[
W = W(h, P) = \mathbf{\hat{W}(h)} + P(h_3 - 1)
\]

(12)

From equation (11), it follows that:

\[
\frac{\partial W}{\partial g} = \mathbf{\hat{S}} = \mathbf{\hat{S}} + G^{-1}p
\]

(13)

Further, we define the Jaumann stress \( \mathbf{\tau} \), as derivable from equation (12) as:

\[
\mathbf{\tau} = \mathbf{\hat{S}} = \frac{\partial W}{\partial h} + (I + h) \mathbf{\hat{S}}
\]

(14)

From equations (13) and (14) it is seen that:

\[
\mathbf{\tau} = \frac{1}{2} [\mathbf{\hat{S}} (I + h) + (I + h) \mathbf{\hat{S}}]
\]

(15)

For completeness, we note that the first Piola–Kirchhoff stress \( \mathbf{\tau} \) is derivable from \( W \), as:

\[
\mathbf{\tau} = \frac{\partial W}{\partial g} T
\]

(16)

Finally, using equation (10) in equation (15), we note that:

\[
\mathbf{\tau} = \frac{1}{2} [\mathbf{\hat{S}} + \mathbf{g} T T]
\]

(17)

Incremental equation strategies for numerical modelling

As is now well recognized, the finite element method offers a simple way to solve the nonlinear problems of the present type. For nonlinear elasticity problems as in the present case, these numerical methods can be formulated so that the fully nonlinear problem is solved in a single step (so that the prescribed total loads or total displacements are applied in a single step); or the problem can be solved incrementally with piecewise linear incremental solutions. Because of their intuitive appeal, and easiness of the solution procedure, incremental approaches are generally preferred; and are considered in the present paper. Again, the incremental method can be either of a stationary Lagrangean type, or of an updated Lagrangean type; in the former method all the state variables in each successive increment are referred to the initial undeformed configuration, while in the later method the state variables in the immediately preceding step. For reasons of simplicity we employ the stationary Lagrangean approach in the present paper. We consider the generic case of an increment from state \( C_N \) to \( C_{N+1} \) which are the states prior to, and after the addition of the \((N + 1)\)th load increment, respectively. The state \( C_N \)

\[
\mathbf{\hat{S}} = \mathbf{\hat{S}}^T
\]

(19)

(Rotational equilibrium)

\[
\mathbf{\hat{g}} = \frac{1}{2} [\mathbf{\hat{S}} \mathbf{\hat{u}} + (\mathbf{\hat{S}} \mathbf{\hat{u}})^T + (\mathbf{\hat{S}} \mathbf{\hat{u}})^T (\mathbf{\hat{S}} \mathbf{\hat{u}}) + (\mathbf{\hat{S}} \mathbf{\hat{u}})^T (\mathbf{\hat{S}} \mathbf{\hat{u}})]
\]

(20)

(Strain displacement rate relation)

\[
\mathbf{\eta} = \mathbf{\hat{S}}^T (\mathbf{\hat{u}})^T + \mathbf{\hat{S}} \mathbf{\hat{u}}^N T = \Delta \mathbf{\hat{t}} = \Delta \mathbf{\tau} \text{ on } S_{\text{u_0}}
\]

(21)

(Traction boundary condition)

\[
\mathbf{\hat{u}} = \tilde{\mathbf{u}} \text{ on } S_{\text{u_0}}
\]

(22)

(Displacement boundary condition)

In terms of \( \mathbf{\hat{g}}, \mathbf{\hat{u}}, \mathbf{\hat{t}} \)

\[
\mathbf{\nabla} \cdot \mathbf{\hat{g}} + \rho_0 \mathbf{\hat{g}} = 0
\]

(23)

(Translational equilibrium)

\[
\mathbf{\hat{g}} = \mathbf{\hat{u}}
\]

(25)

(Translation equilibrium)

\[
\mathbf{\eta} \cdot \mathbf{\hat{t}} = \Delta \mathbf{\hat{t}} \text{ on } S_{\text{u_0}}
\]

(26)

(Displacement boundary condition)

\[
\mathbf{\hat{u}} = \tilde{\mathbf{u}} \text{ on } S_{\text{u_0}}
\]

(27)

In the above \( \rho_0 \) is mass density per unit initial volume; \( \mathbf{\hat{g}} \) is increment in body force from \( C_N \) to \( C_{N+1} \) per unit mass, \( S_{\text{u_0}} \) and \( S_{\text{u_0}} \) are respectively the boundary segments in the initial configuration over which forces and displacements are prescribed. In addition, it can easily be seen that potentials \( \mathbf{W}, \tilde{\mathbf{u}} \) and \( \mathbf{\hat{V}} \) exist such that:

\[
\mathbf{\hat{W}} = \frac{\partial \mathbf{W}}{\partial \mathbf{\hat{g}}}
\]

(28)

\[
\mathbf{\hat{U}} = \frac{\partial \mathbf{\hat{U}}}{\partial \mathbf{\hat{g}}}
\]

(29)

\[
\mathbf{\hat{V}} = \frac{\partial \mathbf{\hat{V}}}{\partial \mathbf{\hat{g}}}
\]

(30)
Equations (28) and (29) are taken as rate constitutive relations for the nonlinear elastic solid. Moreover, the kinematic constraint of incompressibility can be written in rate form as:

$$\frac{\partial f_{i3}}{\partial g} : \dot{g} = 0 \quad (31)$$

or

$$\frac{\partial h_{i3}}{\partial h} : \dot{h} = 0 \quad (32)$$

where \( N \) indicates the value of the indicated derivative at \( C_N \).

In the following we assume the validity of the hypothesis of isotropy for simplicity and reasons of space, without loss of generality. Thus we write \( W \) in equations (11) and (12) as \( W = W(I_1, I_2) \). It can then be shown\(^{10}\) that the potential \( W \) for \( \dot{S} \) can be written as:

$$\dot{W} = \dot{W} + P \frac{\partial f_{i3}}{\partial g} : \dot{g} \quad (33)$$

Likewise, the potential \( \dot{V} \) for the Jaumann-stress rate (referred to \( C_0 \)) can be written as:

$$\dot{V} = \dot{V} + P \frac{\partial h_{i3}}{\partial h} : \dot{h} \quad (35)$$

where:

$$\dot{V} = \dot{V} + P \frac{\partial h_{i3}}{\partial h} : \dot{h} \quad (36)$$

Based on the above considerations, it can be shown that the rate form of all the field equations and boundary conditions in terms of \( S, g \) and \( u \), viz., equations (18–22, 28), can be derived from the stationarity condition of the following general variational functional, which is analogous to the well-known form in linear elasticity generally attributed to Hu and Washizu. This general variational principle is stated as \( \delta \pi = 0 \) where:

$$\pi(\dot{S}, \dot{g}, \dot{u}) = \sum_{V_{om}} \int \{ \dot{W} - \rho_0 \dot{g} \cdot \dot{u} + \frac{1}{2} (\dot{V}u^T : [\dot{S}]^N) - \dot{S} : [\dot{g} - \frac{1}{2} (\dot{V}u^T + (\dot{u}u)^N)^T \dot{V}u^T + (\dot{u}u)^N] \} dV$$

$$- \sum_m \int \dot{S} : \dot{u} dS - \sum_m \int \dot{S} : (\dot{u} - \dot{u}) dS \quad (37)$$

where \( W \) as defined in equations (33) and (34), \( V_{om} \) represents the domain of the solid in initial configuration, and \( S_{om} \) and \( S_u \) are boundary segments in the initial configuration over which tractions and displacements, respectively, are prescribed. The summation sign \( \Sigma \) indicates the sum of the respective integral over the finite number of finite elements, \( m = 1, \ldots, M \) into which the material is considered to be discretized. Also, the variational principle \( \delta \pi = 0 \), for \( \pi \) stated in equation (37), leads to the necessary field equations and boundary conditions, (equations 18–22, 28), and in addition the interelement traction reciprocity condition only when the admissible displacement field \( \dot{u} \) is such that it satisfies a priori the condition of continuity at the interelement boundaries. In some cases, it may be preferable to relax this condition on the displacement field, through the mechanism of Lagrange multipliers, which leads to more versatile hybrid and mixed-hybrid finite element methods (see reference 7 for a detailed discussion). If equation (20) is assumed to be satisfied a priori, and the constitutive law, equation (28), is valid, one can eliminate \( \dot{S} \) and \( \dot{g} \) as variables in equation (37), thus leading to a more familiar rate form of minimum potential energy principle for small deformations superimposed on a finitely deformed stable configuration.

This potential energy principle can thus be stated as \( \delta \pi = 0 \), where:

$$\pi_{\pi}(\dot{u}, \dot{P}) = \sum_m \int \left( \frac{V}{2} \frac{\partial^2 \dot{W}}{\partial g^2} : \dot{g} + P \frac{\partial^2 h_{i3}}{\partial h^2} \right) dV - \sum_m \int \dot{S} : \dot{u} dS \quad (38)$$

where \( \dot{W} \) is related to \( \dot{u} \) through equation (20), and in addition \( \dot{u} \) satisfies equation (22) and the interelement continuity condition a priori. Rather simple finite element methods for incompressible nonlinear elastic materials can be constructed based on the rate principle corresponding to equation (38). An equivalent principle governing the one-step solution (for the entire load being considered as applied in a single step), as opposed to the presently discussed rate formulation, was discussed and applied by Oden.\(^{11}\)

It should be noted that the principles corresponding to equations (37) and (38) only govern the piecewise linear incremental solutions. However, to keep the path of this piecewise linear solution from straying too much from the truly nonlinear hypothetical solution, it is often necessary to employ corrective iterations at the end of each increment. Details of such iterations, and consistent ways to formulate them, can be found elsewhere.\(^{7–9}\)

As is well known, the solutions for stresses obtained by a finite element based on assumed compatible displacements, and application of potential energy rate principles such as in equation (38), are, in general, somewhat unsatisfactory. Often, in the analysis of nonlinear elastic materials such as biological materials, the interest may be more in obtaining a more accurate stress solution rather than the deformation solution. In such cases it is preferable to formulate an assumed stress finite element method based on a complementary rate principle if possible.

It is impossible to derive a rational and consistent complementary energy rate principle involving \( \dot{S} \) or \( \dot{f} \). Recent investigations by the first two authors\(^{8–9}\) indicate that the only rational and practically useful form of a complementary energy rate principle is the one based on the rate of Jaumann stress and the rate of rotation tensor. Note that the rate of Jaumann stress itself is related to the rate of the first Piola–Kirchhoff stress and rate of rotation, through the equation:

$$\dot{I} = \frac{1}{2} I^N + \dot{I}^N \cdot \dot{g} + \dot{g}^T \cdot \dot{I}^N + \dot{g}^N \cdot \dot{I}^T \quad (39)$$
In this approach, the assumed field for the rate of first Piola-Kirchhoff stress satisfies only the translational equilibrium equations, equation (23), which are linear. The rotational equilibrium conditions, equation (24), follow as the Euler equations corresponding to the vanishing of the first variation of the functional, for the complementary energy principle stated below, due to arbitrary variations in the assumed rate of rotation field, \( \dot{\alpha} \). In addition, in the rigorous application of the complementary energy principle to a finite element model of the material, the assumed rate of first Piola-Kirchhoff stress, \( \dot{\sigma} \), must, a priori, satisfy the condition of interelement traction reciprocity (or Newtonian law of equality of action and reaction). To remove this restriction on the chosen \( \dot{\sigma} \), this interelement traction reciprocity is introduced as a constraint condition into the complementary energy rate principle, through Lagrange multipliers, \( \lambda_{om} \), assumed only at the interelement boundary, \( \rho_{om} \). Based on these considerations, it has been shown\(^9\) that the only possible consistent form of a modified complementary energy rate principle for the analysis of incompressible nonlinear elastic solids is given by \( \delta \pi_{HS} = 0 \), where:

\[
\pi_{HS}(\dot{\sigma}, \dot{\alpha}, \dot{u}_p, \dot{P}) = \sum_{m} \int_{V_m} \left[ \left( \frac{\partial \dot{\sigma}^*}{\partial \dot{\alpha}} - (I + h_N^N) \right) \cdot \dot{\alpha} \right] \, dV - \sum_{m} \int_{V_{om}} \left( h_N^N - 1 \right) \dot{P} \cdot (I + h_N^N) \, dV + \tau^{NT} \cdot [\alpha \cdot (I + h_N^N)] \, dV - \sum_{m} \int_{S_{om}} \gamma^N \cdot (\dot{t}^N + I) \cdot (\dot{u}_p^N + \dot{u}_p) \, dS + \sum_{m} \int_{S_{om}} (\dot{t}^N + I) \cdot (\dot{u}_c^N + \dot{u}_c) \, dS \tag{40}
\]

In the above:

\[
\dot{\alpha} = \dot{\sigma} - \frac{\partial h_3}{\partial \dot{h}} \left| ^N \right. \tag{41}
\]

which has the potential \( \dot{V}^* \) such that:

\[
\dot{\dot{r}} = \frac{\partial V^*}{\partial \dot{h}}; \quad \dot{\dot{r}} = \frac{1}{2} \dot{h} \left( \frac{\partial^2 W^*}{\partial h^2} \right) = \frac{\partial^2 h_3}{\partial h^2} \left| ^N \right. \frac{\partial P}{\partial h} \left| ^N \right. \dot{h} \tag{42}
\]

The energy density function \( \dot{R}^* \) in equation (40) is derived through a contact transformation on \( \dot{V}^* \), so that:

\[
\dot{R}^* (\dot{\alpha}) = \dot{h} \cdot \dot{\alpha} - \dot{V} \tag{43}
\]

Finally, the symbol \( V_{om} \) in equation (40) denotes the boundary of the \( m \)th finite element in the initial configuration. Successful first applications of the principle in equation (40) to nonlinear elastic incompressible solids have been given by Murakawa and Atluri.\(^9\)

Conclusions

In the above, consistent, rigorous formulations for numerical analysis of soft biological materials characterized as nonlinear elastic incompressible solids are given. Space limitations preclude the discussion of details of these finite element methods, and the results obtainable from them. The details of the finite element methods along with numerous results of application can be found elsewhere,\(^9,10\) and some of these are included as part of the oral presentation of this paper.

Acknowledgements

The authors gratefully acknowledge the partial support provided for this work by the National Science Foundation, under grant ENG74-21346 and by Georgia Institute of Technology.

References

2. Pinto, J. and Fung, Y. C. J. Biomech. 1973, 6, 597