COMPUTATIONAL MODELLING OF SOME PROBLEMS OF ELASTICITY AND VISCOELASTICITY WITH INDUSTRIAL APPLICATIONS

Simon Shaw, M.K. Warby and J.R. Whiteman

BICOM, Brunel University, Uxbridge, UK

ABSTRACT

The reliability of computational models of physical processes has received much attention in recent years and involves issues such as the validity of the mathematical models being used, the error in any data that the models need, and the accuracy of the numerical schemes being used. These issues are considered in the context of elastic and hyperelastic deformation, when finite element approximations are applied. Goal oriented techniques using specific quantities of interest (QoI) are used for estimating discretisation and modelling errors.

The computational modelling of the rapid large inflation of hyperelastic circular sheets modelled as axisymmetric membranes is treated, with the aim of estimating engineering QoI and their errors. Fine (involving inertia terms) and coarse (quasi-static) models of the inflation are considered. The techniques are applied to thermoforming processes where sheets are inflated into moulds to form thin-walled structures. Current work extending the modelling to thermoplastic materials (ie biomaterials) is discussed, particularly from the aspect of reliability.

Key words: Elasticity, Viscoelasticity, Hyperelasticity, Finite element modelling, Goal oriented methods, Thermoforming

INTRODUCTION

The process of computational modelling for problems of continuum mechanics consists of two main phases. The mathematical model of the physics (reality) has first to be defined, after which a numerical approximation of the model has to be derived and solved to give a numerical solution in terms of quantities of interest (QoI). As each of these phases introduces error, in addition to any error in the data of the problem, the *reliability* of the process is acknowledged to be of great importance. The process of assessment of the error in the mathematical model, modelling error, is called *validation*, whilst that of the error in the numerical approximation is *verification.* Reliability is directly related to *validation* and *verification* (V & V) and is increasingly being studied; see e.g. Babuška et al. [1] and Babuška et al. [2].

In this short review paper we consider computational modelling of a number of problems of elasticity, hyperelasticity and viscoelasticity using finite element methods. Thinking first of *verification* we present various *a priori* error analyses and *a posteriori* error estimators, with references to papers where these have been derived. These are followed by brief descriptions of a number of applications, with numerical results for the QoI. The *validation* of the models in the context of some of these applications is then addressed using goal oriented techniques as proposed by Oden and Prudhomme [3] and applied by Shaw et al. in [4].

The "industrial" applications for which we seek numerical solutions later involve large deformation so that the mathematical models are nonlinear. In order to lead up to computational models for these, in the next section we proceed first with a framework for describing deformation and defining our notation, and then progress to hyperelastic (large) deformation, viscoelasticity, finite viscoelasticity.

Following the applications we consider the successes and limitations of the computational modelling of some industrial problems.

MATHEMATICAL MODELS, WEAK FORMULATIONS AND FINITE ELEMENT METHODS

Solid Mechanics Framework (Small Displacement Case)

Let $\mathcal{G}$ be a compressible solid body with mass density ρ which in its undeformed state occupies the open bounded domain $\Omega\subset\mathbb{R}^n, n = 2,3$ with polygonal/polyhedral boundary $\partial\Omega$. A point in $\bar{\Omega}\equiv\Omega\bigcup\partial\Omega$ is denoted by $\boldsymbol{x}\equiv\left(x_i\right)_{i=1}^{3}$, when n=3. The boundary $\partial\Omega$ is partitioned into disjoint subsets Γ_D and Γ_N such that $\partial\Omega\equiv\Gamma_D\bigcup\Gamma_N$, $\Gamma_D\cap\Gamma_N=\varnothing$ and meas $\left(\Gamma_D\right)>0$.

Suppose that, for time $t\in I\equiv\left(0,T\right]$, $T>0$, the body $\mathcal{G}$ is acted upon by body forces $\boldsymbol{f}\left(x,t\right)\equiv\left(\boldsymbol{f}_i\left(\boldsymbol{x},t\right)\right)_{i=1}^{3}$ for $\boldsymbol{x}\in\Omega$ and surface tractions $\boldsymbol{g}\left(\boldsymbol{x},t\right)\equiv\left(g_i\left(\boldsymbol{x},t\right)\right)_{i=1}^{3}$ for $\boldsymbol{x}\in\Gamma_{\boldsymbol{N}}$. The displacement at a point $\boldsymbol{x}$ under the action of the forces $\boldsymbol{f}$ and $\boldsymbol{g}$ is $\boldsymbol{u}\equiv\left(u_i\left(x,t\right)\right)_{i=1}^{3}$, $\boldsymbol{x}\in\Omega$, $t\in I$, and with a small displacement assumption $\boldsymbol{x}+\boldsymbol{u}\approx\boldsymbol{x}$, so that we do not need to distinguish between the deformed and undeformed domains in most terms. Let $\underline{\boldsymbol{\sigma}}\equiv\left(\sigma_{ij}\right)_{i,j=1}^{3}\equiv\left(\sigma_{ij}\left(\boldsymbol{x},t\right)\right)_{i,j=1}^{3}$ denote the stress resulting from the deformation.

Applying Newton's second law of motion, relating force to the rate of change of linear momentum, to this configuration we obtain the momentum equations

$$\rho\left(\boldsymbol{x}\right)\ddot{u}_i\left(\boldsymbol{x},t\right)-\sigma_{ij,j}\left(\boldsymbol{x},t\right)=f_i\left(\boldsymbol{x},t\right),\quad i=1,2,3 \text{ in } \Omega\times I \tag{1}$$

and these together with the boundary and initial conditions

$$u_i\left(\boldsymbol{x},t\right)=0 \text{ in } \Gamma_D\times\bar{I} \tag{2}$$

$$\sigma_{ij}\hat{n}_j=g_i\left(\boldsymbol{x},t\right), \text{ in } \Gamma_N\times\bar{I} \tag{3}$$

$$u_i\left(\boldsymbol{x},0\right)=u_i^0\left(\boldsymbol{x}\right),\boldsymbol{x}\in\Omega, \tag{4}$$

$$\dot{u}_i(\boldsymbol{x},0) = u_i^1(\boldsymbol{x}), \boldsymbol{x} \in \Omega, \tag{5}$$

define the *dynamic* deformation problem, where $\hat{\boldsymbol{n}} \equiv (\hat{n}_i)_{i=1}^n$ is the unit outward normal to Γ_N, the Einstein convention has been used, and $v,_j \equiv \partial v / \partial x_j$.

If the inertia terms can be neglected in the deformation and assuming that $\boldsymbol{u} = 0 \quad \forall t < 0,$ we obtain the quasistatic problem, where $i, j = 1,2,3,$

$$-\sigma_{ij,j}(\boldsymbol{x},t) = f_i(\boldsymbol{x},t), \text{ in } \Omega \times I \tag{6}$$

$$u_i(\boldsymbol{x},\boldsymbol{t}) = 0, \text{ in } \Gamma_D \times \overline{I} \tag{7}$$

$$\sigma_{ij}\hat{n}_j = g_i(\boldsymbol{x},t), \text{ in } \Gamma_N \times \overline{I}, \tag{8}$$

In order to complete the definitions of the dynamic and quasistatic problems it is necessary to have a constitutive relationship connecting the stress to the displacement and its derivatives.

The constitutive relationship reflects the behaviour of the material of the body $\mathcal{G}$.

Linear elasticity and weak formulation

In the case of small displacement gradients the strain is described by the infinitesimal strain tensor $\underline{\boldsymbol{\varepsilon}}(\boldsymbol{u}) \equiv (\varepsilon_{ij}(\boldsymbol{u}))_{i,j=1}^n$ as

$$\varepsilon_{ij}(\boldsymbol{u}) = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \; i, j = 1,2,3. \tag{9}$$

For an isotropic linear elastic material Hooke's law connects stress to strain (i.e. to the derivatives of the displacement) and we have

$$\sigma_{ij} = \lambda \nabla.\boldsymbol{u}\delta_{ij} + \mu\varepsilon_{ij}(\boldsymbol{u}), \tag{10}$$

where δ_{ij} is the Kronecker delta, and λ and μ are the Lamé coefficients of the material. More generally the relation for a linear elastic material can be written in the form

$$\underline{\boldsymbol{\sigma}} = \underline{\boldsymbol{D}}\boldsymbol{\varepsilon}. \tag{11}$$

We note that elasticity is a time independent phenomenon, so that the mathematical model for linear elasticity is based on equations (6), (7), (8) and (10) with $\boldsymbol{u}(\boldsymbol{x},t)$ depending only on quantities at time *t*.

In order to obtain a weak form from these equations we introduce the usual Sobolev spaces $H^r(\Omega), r = 0,1,\ldots,$ and for $V_1, V_2, \ldots, V_n \subset H^r(\Omega)$ we define the space *V*, such that

$$\begin{aligned} V &\equiv V_1 \times V_2 \times \ldots \times V_n \\ &\equiv \left\{\boldsymbol{v} \in \left(H^1(\Omega)\right)^n : \boldsymbol{v} = 0 \text{ on } \Gamma_D\right\}. \end{aligned} \tag{12}$$

Multiplying (6) by a test function $\boldsymbol{v} \in V,$ and integrating by parts over Ω we obtain

$$\int_\Omega \sigma_{ij}(\boldsymbol{u})\varepsilon_{ij}(\boldsymbol{v})d\Omega = (\boldsymbol{f},\boldsymbol{v})_\Omega + (\boldsymbol{g},\boldsymbol{v})_{\Gamma_N}, \tag{13}$$

where the (.,.) are inner products. Applying Hooke's law (10) we obtain the weak form of the isotropic linear elasticity problem: find $\boldsymbol{u} \in V$ such that

$$a(\boldsymbol{u},\boldsymbol{v}) = L(\boldsymbol{v})\,\forall \boldsymbol{v} \in V,$$

where
$$a(\boldsymbol{v},\boldsymbol{w}) \equiv \int_{\Omega} \lambda \nabla.\boldsymbol{v}\nabla.\boldsymbol{w} + \mu\varepsilon_{ij}(\boldsymbol{v})\varepsilon_{ij}(\boldsymbol{w})\,d\Omega, \tag{14}$$

$$L(\boldsymbol{v}) \equiv \int_{\Omega} f_i v_i \partial\Omega + \int_{\Gamma_N} g_i v_i d\Gamma,\; i,j = 1,2,3.$$

In order to apply the finite element method to problem (14), we first partition Ω into a set of elements $\left\{\Omega_i^h\right\}_{i=1}^{N_E}$, where $\bar{\Omega}^h \subset \bar{\Omega} = \bigcup_i \Omega_i^h$ and $\partial\Omega^h \equiv \partial\Omega,$ each with diameter h_i and define $h \equiv \underset{1 \leq i \leq N_E}{max}\, h_i$ We construct finite dimensional spaces

$V_i^h \equiv$ span $\left\{\Phi_i(\boldsymbol{x})\right\}_{i=1}^{N_N} \subset V_i,$ for $1 \leq i \leq n$ with each $\Phi_i \in \mathbb{P}^r$,a piecewise polynomial of

degree r over the partition, where the $\Phi_i(\boldsymbol{x})$ are basis functions associated with the N_N nodes of the partition. Finally we define

$$V^h \equiv V_1^h \times V_2^h \times \ldots \times V_n^h \subset V$$

The finite element problem is: find $\boldsymbol{u_h} \in V^h$ such that

$$a(\boldsymbol{u}_h,\boldsymbol{v}_h) = L(\boldsymbol{v}_h)\;\; \forall \boldsymbol{v}_h \in V^h. \tag{15}$$

There is a vast literature associated with the derivation of *a priori* estimates for the error $\boldsymbol{e}_h \equiv (\boldsymbol{u} - \boldsymbol{u}_h)$ of the form

$$\|\boldsymbol{e}_h\|_{\alpha,\Omega} \leqq \mathcal{C}\, h^{\beta(\alpha,r)} |\boldsymbol{u}|_{r,\Omega}, \tag{16}$$

where $\| \;\|_{q,\Omega}$ is the norm on $H^q(\Omega)$; see e.g. Ciarlet [5], Oden and Reddy [6] and Whiteman

[7]. In (16) the function $\beta(\alpha,r)$ depends on the regularity of the solution $\boldsymbol{u}$ of (14) and $\mathcal{C}$ is

a constant that depends on α but is independent of $\boldsymbol{u}$ and the mesh. Estimates of this type provide rates of convergence of $\boldsymbol{u_h}$ to $\boldsymbol{u}$ with decreasing mesh size h.

Similarly many *a posteriori* error estimators, (i.e. calculable error estimators involving the calculated solution $\boldsymbol{u}_h$) and based for example on residuals $R(\boldsymbol{v})$ of the type

$$R(\boldsymbol{v}_h) = \sum_{i=1}^{N_E} L(\boldsymbol{u}_h) - a(\boldsymbol{u}_h,\boldsymbol{v}_h), \tag{17}$$

have now been derived, see e.g. Oden and Ainsworth [8] and Babuska et al [2], and again the performance of these depends on the regularity of $\boldsymbol{u}$. The process of verification is made possible by the use of estimates of the type of (16) and (17).

Large Deformation Elasticity

Motivated by the problem of the large deformation of a thin polymer sheet that will be considered later, we now describe the large elastic deformation under the action of applied

pressure loading for the case of an elastic sheet, $\mathcal{B}$, using a Lagrangian description. Again

$\boldsymbol{x}$ denotes a point in the body which in the deformation undergoes a displacement $\boldsymbol{u}$ so that $\boldsymbol{x} \rightarrow \boldsymbol{x} + \boldsymbol{u} \equiv \boldsymbol{w}.$ In the large deformation case $\boldsymbol{u}$ and the displacement gradient are no longer small so that care is needed to distinguish between the undeformed and the deformed states. An outcome of this in the description of the deformation is to introduce the nominal stress $\underline{\Pi} \equiv \left(\det \underline{\boldsymbol{F}}\right) \underline{\boldsymbol{F}}^{-1} \underline{\boldsymbol{\sigma}},$ where $\underline{\boldsymbol{F}} \equiv \left(\partial w_i / \partial x_j\right),\ j = 1,2,3$ is the deformation gradient and, as before, $\boldsymbol{\sigma}$ is the Cauchy stress.

The equations of equilibrium of a body undergoing large elastic deformation, corresponding to (6) for small deformation, can for the three-dimensional case be written as

$$-\sum_{j=1}^{3} \frac{\partial \Pi_{ij}}{\partial x_j} = f_i \qquad i = 1,2,3. \tag{18}$$

The problem that we shall consider involves the large deformation of a thin sheet, with mid-surface $\Omega,$ which is clamped on the boundary Γ of Ω and which in its undeformed state has thickness $h_0.$ The sheet occupies the region

$$\mathcal{B} \equiv \left\{ \left(x_1, x_2, x_3\right) : \boldsymbol{x} = \left(x_1, x_2\right)^T \in \Omega, \left|x_3\right| < h_0 / 2 \right\}. \tag{19}$$

Now $x_3 = 0$ on the mid-surface $\Omega,$ which deforms as $\left(x_1, x_2, 0\right) \rightarrow \left(x_1 + u_1, x_2 + u_2, u_3\right),$ and, assuming that normals to Ω remain normal, we obtain a two-dimensional description of the sheet with $\boldsymbol{u} = \boldsymbol{u}\left(\boldsymbol{x}\right).$ The sheet is modelled as a membrane, thus being unable to support bending so that $\underline{\boldsymbol{\sigma}}.\boldsymbol{n} = 0,$ where $\boldsymbol{n}$ is the unit normal to the deformed mid-surface $\Omega.$

In this context of a membrane approximation to the general three-dimensional case, the two-dimensional equations for the problem, when there is a pressure loading P and assuming that the body forces $\boldsymbol{f}$ are zero, lead to the weak form of (18): find $\boldsymbol{u} \in V$ such that

$$a\left(\boldsymbol{u};\boldsymbol{v}\right) = 0 \quad \forall \boldsymbol{v} \in V, \quad a\left(\boldsymbol{u};\boldsymbol{v}\right) = a_1\left(\boldsymbol{u};\boldsymbol{v}\right) - P a_2\left(\boldsymbol{u};\boldsymbol{v}\right), \tag{20}$$

where

$$a_1\left(\boldsymbol{u};\boldsymbol{v}\right) \equiv \int_\Omega h_0 \left(\Pi^T : \nabla \boldsymbol{v}\right) d\Omega, \tag{21}$$

$$a_2\left(\boldsymbol{v};\boldsymbol{w}\right) \equiv \int \boldsymbol{v}.\left(\frac{\partial \boldsymbol{w}}{\partial x_1} \times \frac{\partial \boldsymbol{w}}{\partial x_2}\right) d\Omega, \tag{22}$$

and now the space $V \equiv V_1 \times V_2$ is such that

$$V \equiv \left\{ \boldsymbol{v} \in \left(H^1\left(\Omega\right)\right)^2 : \boldsymbol{v} = 0 \text{ on } \Gamma \right\}. \tag{23}$$

The finite element method is applied to obtain an approximation $\boldsymbol{u}_h$ to $\boldsymbol{u}$ the solution of (20) for the case of incremental loading of the sheet. As we have a Lagrangean description of the deformation, the spatial mesh is defined on the reference configuration $\Omega \subset \mathbb{R}^2$ and, for each load increment P_j, the nonlinear system

$$a_1(\boldsymbol{u}_h;\boldsymbol{v}_h) - P_j a_2(\boldsymbol{u}_h;\boldsymbol{v}_h) = 0 \quad \forall \boldsymbol{v}_h \in V^h, \tag{24}$$

is solved for $\boldsymbol{u}_h \in V^h$ using Newton's method, where $V^h \equiv V_1^h \times V_2^h \subset V$ and the $V_i^h, i = 1,2$ are spaces of piecewise polynomial functions defined over the partition of Ω, see e.g. Karamanou et al. [8].

For the problem (20), noting that $a(\boldsymbol{u};\boldsymbol{v})$ is a semilinear form (i.e. linear in arguments to the right of the semi-colon), we suppose that we wish to approximate the quantity of interest $J(\boldsymbol{u}), \boldsymbol{u} \in V$ with $J(\boldsymbol{u}_h), \boldsymbol{u}_h \in V^h$.

If $a'(.\,;.)$ and $J'(.\,;.)$ are Gateaux derivatives of $a(.\,;.)$ and $J(.\,;.)$ respectively then, if $\boldsymbol{e}_h = \boldsymbol{u} - \boldsymbol{u}_h$,

$$J(\boldsymbol{u}) - J(\boldsymbol{u}_h) = \int_0^1 J'(\boldsymbol{u}_h + s\boldsymbol{e}_h;\boldsymbol{e}_h)ds \tag{25}$$

and

$$\begin{aligned} -a(\boldsymbol{u}_h;\boldsymbol{z}) &= a(\boldsymbol{u};\boldsymbol{z}) - a(\boldsymbol{u}_h;\boldsymbol{z}) \\ &= \int_0^1 a'(\boldsymbol{u}_h + s\boldsymbol{e}_h;\boldsymbol{e}_h,\boldsymbol{z})ds. \end{aligned} \tag{26}$$

If we now consider the (dual) linear problem find $\boldsymbol{z} \in V^h$ such that

$$\int_0^1 a'(\boldsymbol{u}_h + s\boldsymbol{e}_h;\boldsymbol{v}_h,\boldsymbol{z})ds = \int_0^1 J'(\boldsymbol{u}_h + s\boldsymbol{e}_h;\boldsymbol{v}_h)ds \quad \forall \boldsymbol{v}_h \in V^h, \tag{27}$$

then we have a representation of the error as

$$J(\boldsymbol{u}) - J(\boldsymbol{u}_h) = -a(\boldsymbol{u}_h;\boldsymbol{z}). \tag{28}$$

But $\boldsymbol{z}$ depends on $\boldsymbol{u}$ so that (27) cannot be solved as it stands and some form of approximation has to be adopted. One strategy for this is to apply the left hand rule for the integration giving

$$a'(\boldsymbol{u}_h;\boldsymbol{v}_h,\hat{\boldsymbol{z}}) = J'(\boldsymbol{u}_h;\boldsymbol{v}_h), \quad \forall \boldsymbol{v}_h \in \tilde{V}^h, \tag{29}$$

where $\tilde{V}^h \subset \hat{V}^h$, giving the estimate

$$J(\boldsymbol{u}) - J(\boldsymbol{u}_h) \approx -a(\boldsymbol{u}_h,\hat{\boldsymbol{z}}). \tag{30}$$

This "machinery" for estimating the discretisation error will be referenced for a problem of free inflation of a thin polymer sheet in a later section.

We have so far treated only discretisation error. In order to consider modelling error we introduce the concept of *fine* and *coarse* problems in the context of the deformation of the sheet. For example the problem (20) which is quasi-static could be taken as a coarse problem and the fine problem could be similar, but with the inclusion of inertia terms in (18). In many practical situations it is not clear whether inertia terms are important to the modelling. Suppose therefore that the fine problem has the weak form

$$A(\boldsymbol{U};\boldsymbol{v}) = 0 \quad \forall v \in V, \tag{31}$$

where the semilinear form $A(.\,;.)$ contains the $a_1(.\,;.)$ and $a_2(.\,;.)$ of (20) and the inertia terms. The dual approximating problem corresponding to (29) is now

$$A'(\boldsymbol{u}_h;\boldsymbol{v}_h,\hat{\boldsymbol{z}}) = J'(\boldsymbol{u}_h;\boldsymbol{v}_h) \quad \forall \boldsymbol{v}_h \in \tilde{V}^h, \tag{32}$$

where the $\boldsymbol{u}_h$ is the solution of the coarse problem and now $\tilde{V}^h \subset V$ is an appropriate finite dimensional space. We now have the estimate

$$J(\boldsymbol{U}) - J(\boldsymbol{u}_h) \approx -A\left(\boldsymbol{u}_{h_j}\hat{\boldsymbol{z}}\right)$$

for the combined modelling and discretisation errors. More details of these goal oriented techniques can be found in Shaw et al. [4].

Viscoelasticity

The formation and use of non-metallic materials has been one of the great advances of science, engineering, medicine and manufacturing of recent years. In particular in the context of solids, the development of polymeric materials has been especially significant to advances in the design of structures and the performance of their deformation behaviour. A feature of the deformation of polymeric solid materials is that when they are subjected to sustained loading, in addition to an elastic response, they can exhibit time dependent creep. For example a polymer test specimen subjected to an instantaneously applied and sustained tensile loading will undergo an initial elastic (solid) deformation, followed over time by creep during which the specimen will continue to stretch. Creep is a viscous fluid effect and, due to the dual elastic and viscous responses, materials that exhibit this type of behaviour are said to be **viscoelastic.** If the loading is removed from the solid it will experience an instantaneous elastic recovery followed by a reverse time dependent recovery in which the solid returns to its original state. For this reason viscoelastic solids are said to possess **memory.**

Returning again to the case of small displacements and small strains, we recall that in the case of linear elasticity the constitutive relation was $\underline{\boldsymbol{\sigma}} = \underline{\boldsymbol{D}}\underline{\boldsymbol{\varepsilon}}$ as in (11). Turning now to

viscoelastic deformation of the body $\mathcal{G}$, and assuming this to be both quasistatic and small, the

deformation $\boldsymbol{u}(\boldsymbol{x},t)$ is governed by (6) – (8) for $(\boldsymbol{x},t) \in \Omega \times I$ and the strain $\underline{\boldsymbol{\varepsilon}}$ is as in (9). For linear elasticity the constitutive relation was Hooke's law (11), but in the case of linear viscoelasticity where the materials possess memory, i.e. the current stress depends on the history of the deformation, it is necessary to introduce time dependence and to augment Hooke's law with a memory term. In this way the stress can now be expressed as a linear functional of the strain, so that

$$\underline{\sigma}(\boldsymbol{x},t) = \underline{\boldsymbol{D}}(\boldsymbol{x})\,\underline{\boldsymbol{\varepsilon}}\big(\boldsymbol{u}(\boldsymbol{x},t)\big) - \int_0^t \frac{\partial \underline{\boldsymbol{D}}}{\partial s}(\boldsymbol{x},t-s)\,\underline{\boldsymbol{\varepsilon}}\big(u(\boldsymbol{x},s)\big)\,ds, \qquad (33)$$

where $\underline{\boldsymbol{D}} \equiv \left(D_{ijkl}(\boldsymbol{x})\right)_{i,j,k,l=1}^{n}$ is a fourth order tensor of relaxation functions with components which are assumed to be $C^1(I)$ functions of *t*. At $t = 0$ it is assumed that $\underline{\boldsymbol{\varepsilon}} = 0$.

In order to define a weak formulation of this quasistatic problem we need a test space of admissible functions on $\Omega \times I$ and for this we proceed in two stages. We first multiply by a space only test function and integrate over Ω and then extend the test space and integrate over *I*. Multiplication of (6) by a (space only) function $\boldsymbol{v} \in V$, see (12), produces (13) for any $t \in I$, which on use of (31) leads to the problem: find $\boldsymbol{u} \in L_\infty(I;V)$ such that

$$\tilde{a}\big(\boldsymbol{u}(t),\boldsymbol{v}\big) = \tilde{L}(t;\boldsymbol{v}) + \int_0^t \tilde{b}\big(t,s;\boldsymbol{u}(s),\boldsymbol{v}\big)ds \quad \forall \boldsymbol{v} \in V, \qquad (34)$$

where

$$\tilde{a}(\boldsymbol{w},\boldsymbol{v}) \equiv \int_\Omega D_{ijkl}(0)\,\varepsilon_{kl}(\boldsymbol{w})\,\varepsilon_{ij}(\boldsymbol{v})\,d\Omega, \qquad (35)$$

$$\tilde{b}(t;s;\boldsymbol{w},\boldsymbol{v}) \equiv \int_{\Omega} \frac{\partial D_{ijkl}}{\partial s}(t-s)\,\varepsilon_{kl}(\boldsymbol{w})\,\varepsilon_{ij}(\boldsymbol{v})\,d\Omega \tag{36}$$

for all $\boldsymbol{w},\boldsymbol{v} \in V$ and $\tilde{L} : I \times V \to \mathbb{R}$ is a time dependent linear form as in (14). As (34) contains no time derivative we seek the solution $\boldsymbol{u} \in L_{\infty}(I;V)$ by solving the "fully weak" problem: find $\boldsymbol{u} \in L_{\infty}(I;V)$ such that

$$a(\boldsymbol{u},\boldsymbol{v}) = L(v) \quad \forall v \in L_1(I;V), \tag{37}$$

where

$$a(\boldsymbol{u},\boldsymbol{v}) = \int_0^T \tilde{a}(\boldsymbol{u}(t),\boldsymbol{v}(t))dt - \int_0^T \int_0^t \tilde{b}(t,s;u(s),v(t))dsdt, \tag{38}$$

$$L(\boldsymbol{v}) = \int_0^t L(t;v(t))dt. \tag{39}$$

In order to apply the finite element method to (37) we first split the prismatic domain $\Omega \times I$ into M time slabs $\Omega_i \equiv \Omega \times I_i$ where $I_i = \{(t_{i-1},t_i)\}_{i=1}^{M}$ and partition each of these into M_i elements Ω_{ij} and define for each Ω_i the space

$$H_i \equiv \left\{ \boldsymbol{v} \in V \cap \left(C(\bar{\Omega})\right)^n, \text{ where } v \text{ is linear on } \Omega_{ij} \text{ for each } j = 1,\dots M_i \right\}$$

and hence the space-time finite element spaces $V^{r,h}$, where

$$V^{r,h} \equiv \left\{ \boldsymbol{v} \in L_{\infty}(I;V) : v\big|_{I_i} \in \mathbb{P}(I_i;H_i)\,\forall i = 1,2,3 \right\} \tag{40}$$

Functions in $V^{r,h}$ are continuous in space but usually discontinuous in time.
Many *a priori* error estimates have been derived for this type of finite element discretisation and take the form

$$\left\|\boldsymbol{u} - \boldsymbol{U}_h\right\|_{L_{\infty}(I;V)} \leq \mathcal{C}(T)\left(\Pi_h \left\|hD^2\boldsymbol{u}\right\|_{L_{\infty}(I;L_2(\Omega))} + \Pi_k \left\|\frac{k^{r+1}\partial^{r+1}\boldsymbol{u}}{\partial t^{r+1}}\right\|_{L_{\infty}(I;V)}\right), \tag{41}$$

where $\boldsymbol{U}_h$ denotes the finite element approximation, $\mathcal{C}$(T) is a stability constant, the Π's are

positive constants and *h* and *k* are maximum values of the space and time mesh lengths respectively. Note that the right hand side of (39) contains, as might be expected, a space and a time term. Further details can be found in Shaw and Whiteman [9] and [10] and Riviére et al. [11].

As viscoelastic materials display characteristics of both elastic solids and viscous fluids, many models involving combinations of springs and dashpots have been proposed, for example the Maxwell solid model, see e.g. Ferry [12]. For these cases the stress relaxation functions are represented using Prony series of decaying exponential functions so that the stress in (33) can be expressed in terms of internal variables of the model, for example internal stresses. These internal variables each satisfy ordinary differential equations in time; it is by integrating these ODE's that (33) can be obtained. Thus an alternative approach to the above history integral formulation of the linear viscoelastic problem is to solve a coupled system of PDE's consisting at each time step of an elastic problem of the type as in (14), but with internal variables contained in the right hand side, together with a system of ordinary differential equations in time for the internal variables; see e.g. Shaw et al. [13] where finite element models and error estimates are presented.

The formulation using internal variables has been extended to the case of finite viscoelastic deformation of a thin sheet, motivated by the large elastic deformation model described above using the nominal stress. Thus in this case we have a finite elasticity equation of the type (20) but now involving additional internal variable terms on the right hand side, which is solved coupled to a system of now nonlinear ODE's for the internal variables, see Karamanou [8].

APPLICATION

Thermoforming of Thin Polymer Sheets

We return now to the computational modelling of the large hyperelastic deformation of thin polymeric sheets into moulds as in thermoforming processes. The sheets are clamped at the edges and are acted on by pressure. The deformation has two stages; the first is free inflation prior to contact with mould, the second is inflation after part of the sheet has made contact with the mould. In these processes decisions have to be made as to the form of the deformation (hyperelastic, finite viscoelastic, elasto-plastic, …) and also as to whether the deformation takes place at a rate that causes the inertia terms in the models to be important.

Considering first the free inflation phase, the goal oriented techniques of the Large Deformation Elasticity section of this paper have been applied to the deformation of a circular sheet, modelled as described taking (20) without inertia terms as the coarse model and (31), including inertia terms, as the fine model.

Estimates of both the discretisation error for the finite element approximation of the coarse model and of the combined modelling and discretisation errors for the fine model have been obtained; see [4], and these demonstrate that the method is robust for this free inflation problem under the given conditions.

The second phase of the inflation has in recent years been modelled extensively under the assumptions that the deformation is quasistatic and that perfect sticking of the sheet to the mould takes place on contact, see e.g. Karamanou et al. [8] and Warby et al. [14]. To our knowledge no error estimates have been obtained for this case.

COMMENTS

The application as above demonstrates what error analysis can and cannot do for a problem of thermoforming. It must be emphasised that assumptions have to be made in setting up any mathematical model. These are often based on "best practice" in the industry concerned and cannot be rigorously justified.

Similarly the advent of new materials presents continuing challenges. For example traditionally the polymers used in thermoforming processes have been oil based. With the current move to eco-friendliness the fact that these materials do not biodegrade is significant. As a result biomaterials, thermoplastics, are being used more and more in thermoformed structures. The challenge here is that, for each new material, the material properties have to be found by experiment and they differ significantly from those of the oil based materials. For example the properties of thermoplastic starch depend markedly not only on temperature but also on humidity, see [15].

For these reasons mathematical theory will always lag behind engineering practice.

REFERENCES

[1] Babuška I, Nobile F and Tempone R (2007) Reliability in computational science. Numerical Methods for Partial Differential Equations 23, 753 – 784.

[2] Babuška I, Whiteman J.R. and Strouboulis T. (2010) Finite Elements: An Introduction and a posterior Error Estimation. Oxford University Press

[3] Oden J.T. and Prudhomme S. (2001) Goal-oriented error estimation and adaptivity for the finite element method. Computers and Mathematics with Applications 41, 735 – 756.

[4] Shaw S, Warby M.K. and Whiteman J.R. (2010) Discretization and Modelling error in the context of the rapid inflation of hyperelastic membranes. *IMA Journal of Numerical Analysis*, 302-333.

[5] Ciarlet P.G. (1978) The Finite Element Method for Elliptic Problems. North-Holland, Amsterdam.

[6] Oden J.T. and Reddy J.N. (1976) An Introduction to the Mathematical Theory of Finite Elements. Wiley, New York.

[7] Whiteman J.R. (ed.) (1973) The Mathematics of Finite elements and applications. Academic Press, London.

[8] Karamanou M, Warby M.K. and Whiteman J.R. (2006) Computational modelling of thermoforming processes in the case of finite viscoelastic materials. *Computer Methods in Applied Mechanics and Engineering* 195, 5220-5238.

[9] Shaw S and Whiteman J.R. (2000) Numerical solution of linear quasistatic hereditary viscoelastic problems. *SIAM Journal of Numerical Analysis* 38, 80-97.

[10] Shaw S and Whiteman J.R. (1997) Towards robust adaptive finite element methods for partial differential Volterra equation problems arising in viscoelasticity. In J.R. Whiteman (ed.) The Mathematics of Finite Elements and Applications. Wiley, Chichester, 56 – 80.

[11] Riviere B, Shaw S, Wheeler MF. and Whiteman J.R. (2003) Discontinuous Galerkin finite element method for linear elasticity and quasistatic linear viscoelasticity. *Numerische Mathematik* 95, 347-376

[12] Ferry J.D. (1970) Viscoelastic Properties of Polymers. Wiley, New York.

[13] Shaw S., Warby M.K. and Whiteman J.R. (1997) A comparison of hereditary integral and internal variable approaches to numerical solid viscoelasticity. In Proc. XIII Polish Conf. on Computer Methods in Mechanics. Posnan.

[14] Warby M.K., Whiteman J.R., Jiang W-G, Warwick P, Wright T. (2002) Finite element simulation of thermoforming processes for polymer sheets, *Mathematics and Computers in Simulation*, 2105, 1-10.

[15] Szegda D, Song J, Warby M.K. and Whiteman J.R. (2007) Computational Modelling of a Thermoforming Process for Thermoplastic Starch. American Institute of Physics, Proceedings 908, 35 – 47.