Computational Modelling of Some Problems of Elasticity and Viscoelasticity with Applications to Thermoforming Processes

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Abstract

The reliability of computational models of physical processes has received much attention 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, viscoelastic and hyperelastic deformation, when finite element approximations are applied. Goal oriented techniques using specific quantities of interest (QoI) are described for estimating discretisation and modelling errors in the hyperelastic case.

The computational modelling of the rapid large inflation of hyperelastic circular sheets modelled as axisymmetric membranes is then 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.

Key words: elasticity, viscoelasticity, hyperelasticity, finite element modelling, goal oriented methods, thermoforming

1. 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 problems of elasticity, viscoelasticity and hyperelasticity using finite element methods. Thinking first of *verification* we present various *a priori* error analyses and *a posteriori* error estimators in the contexts of elasticity and viscoelasticity, with references to papers where these have been derived. These are followed by brief descriptions of a hyperelastic application. The *validation* of the models in this context is then addressed using goal oriented techniques as proposed by Oden and Prudhomme [3] and applied by Shaw et al. in [4].

In order to lead up to computational models for these problems, in the next section we proceed first with a framework for describing deformation and defining our notation, then address small displacement elasticity and viscoelasticity, and finally progress to hyperelastic (large) deformation. The last section of the paper deals with the computational modelling of thermoforming processes.

2. Mathematical models, weak formulations and finite element methods

2.1 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 $\bar{\Omega}\equiv\Omega\cup\partial\Omega$ 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 $\partial\Omega\equiv\Gamma_D\cup\Gamma_N$, $\Gamma_D\cap\Gamma_N=\varnothing$ and meas $\left(\Gamma_D\right)>0$. Suppose that, for time $t\in I\equiv(0,T]$, $T>0$, the body $\mathcal{G}$ is acted upon by body forces

$$\boldsymbol{f}(x,t)\equiv\left(\boldsymbol{f}_i(\boldsymbol{x},t)\right)_{i=1}^3,$$

for $\boldsymbol{x}\in\Omega$ and surface tractions

$$\boldsymbol{g}(\boldsymbol{x},t)\equiv\left(g_i(\boldsymbol{x},t)\right)_{i=1}^3,$$

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 $\boldsymbol{u}\equiv\left(u_i(x,t)\right)_{i=1}^3$, $\boldsymbol{x}\in\Omega$, $t\in I$, 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 $\underline{\boldsymbol{\sigma}}\equiv\left(\sigma_{ij}\right)_{i,j=1}^3\equiv\left(\sigma_{ij}(\boldsymbol{x},t)\right)_{i,j=1}^3$ 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

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

and these together with the boundary and initial conditions

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

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

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

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

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 $\boldsymbol{u}(\boldsymbol{x},t) = 0 \forall t < 0.$ 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 $\mathcal{G}$.

2.2 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

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

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 $H^r(\Omega), r = 0,1,...,$ and for $V_1, V_2, ..., V_n \subset H^r(\Omega)$ we define the space *V*, such that

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

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

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

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

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 $h \equiv \max_{1 \le i \le N_E} h_i$ We construct finite dimensional spaces

$V_i^h \equiv \text{span} \left\{\Phi_i(\boldsymbol{x})\right\}_{i=1}^{N_N} \subset V_i,$ for $1 \le i \le n$ 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

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

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

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

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 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

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

have now been derived, see e.g. Oden and Ainsworth [1] 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).

3. 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. 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 asymptotically to its original state. For this reason viscoelastic solids are said to possess *memory*.

Continuing with 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

$$\underline{\sigma}(\boldsymbol{x},t) = \underline{\boldsymbol{D}}(\boldsymbol{x})\underline{\boldsymbol{\varepsilon}}(\boldsymbol{u}(\boldsymbol{x},t)) - \int_0^t \frac{\partial \underline{\boldsymbol{D}}}{\partial s}(\boldsymbol{x},t-s)\underline{\boldsymbol{\varepsilon}}(u(\boldsymbol{x},s))\,ds, \tag{18}$$

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 (18) leads to the problem: find $\boldsymbol{u} \in L_\infty(I;V)$ such that

$$\tilde{a}(\boldsymbol{u}(t),\boldsymbol{v}) = \tilde{L}(t;\boldsymbol{v}) + \int_0^t \tilde{b}(t,s;\boldsymbol{u}(s),\boldsymbol{v})ds \quad \forall \boldsymbol{v} \in V, \tag{19}$$

where

$$\tilde{a}(\boldsymbol{w},\boldsymbol{v}) \equiv \int_\Omega D_{ijkl}(0)\varepsilon_{kl}(\boldsymbol{w})\varepsilon_{ij}(\boldsymbol{v})\,d\Omega, \tag{20}$$

$$\tilde{b}(t;s;\boldsymbol{w},\boldsymbol{v}) \equiv \int_\Omega \frac{\partial D_{ijkl}}{\partial s}(t-s)\varepsilon_{kl}(\boldsymbol{w})\varepsilon_{ij}(\boldsymbol{v})\,d\Omega, \tag{21}$$

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 (19) 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

$$a(\boldsymbol{u},\boldsymbol{v}) = L(v) \quad \forall v \in L_1(I;V), \tag{22}$$

where

$$a(\boldsymbol{u},\boldsymbol{v}) = \int_0^T \tilde{a}(\boldsymbol{u}(t),\boldsymbol{v}(t))dt - \int_0^T \int_0^t \tilde{b}(t,s;u(s),v(t))dsdt, \qquad (23)$$

$$L(\boldsymbol{v}) = \int_0^t L(t;v(t))dt. \qquad (24)$$

In order to apply the finite element method to (22) 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

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

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

$$V^{r,h} \equiv \left\{ \boldsymbol{v} \in L_\infty(I;V) : v\big|_{I_i} \in \mathbb{P}(I_i;H_i) \,\forall i = 1,2,3 \right\}. \qquad (25)$$

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

$$\|\boldsymbol{u} - \boldsymbol{U}_h\|_{L_\infty(I;V)} \leq \mathcal{C}(T)\left(\Pi_h \left\| hD^2\boldsymbol{u} \right\|_{L_\infty(I;L_2(\Omega))} + \Pi_k \left\| \frac{k^{r+1}\partial^{r+1}\boldsymbol{u}}{\partial t^{r+1}} \right\|_{L_\infty(I;V)} \right), \qquad (26)$$

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 (26) 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 [13]. For these cases the stress relaxation functions are represented using Prony series of decaying exponential functions so that the stress in (18) 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 (18) 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. [12] where finite element models and error estimates are presented.

4. Large Deformation Elasticity for Thin Sheets

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 $\boldsymbol{x} \to \boldsymbol{x} + \boldsymbol{u} \equiv \boldsymbol{w}.$ 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 $\underline{\boldsymbol{F}} \equiv \left(\partial w_i / \partial x_j\right)\ i, j = 1,2,3$ 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

$$-\sum_{j=1}^{3} \frac{\partial \Pi_{ij}}{\partial x_j} = f_i \qquad i = 1,2,3. \tag{27}$$

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

$$\mathcal{B} \equiv \left\{ \left(x_1, x_2, x_3\right) : \boldsymbol{x} = \left(x_1, x_2\right)^T \in \Omega, \left|x_3\right| < h_0 / 2 \right\}. \tag{28}$$

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 (27): find $\boldsymbol{u} \in V$ such that

$$a\left(\boldsymbol{u};\boldsymbol{v}\right) = 0 \quad \forall \boldsymbol{v} \in V, \text{ with } \ a\left(\boldsymbol{u};\boldsymbol{v}\right) = a_1\left(\boldsymbol{u};\boldsymbol{v}\right) - P a_2\left(\boldsymbol{u};\boldsymbol{v}\right), \tag{29}$$

where

$$a_1\left(\boldsymbol{u};\boldsymbol{v}\right) \equiv \int_\Omega h_0 \left(\Pi^T : \nabla \boldsymbol{v}\right) d\Omega, \tag{30}$$

$$a_2\left(\boldsymbol{v};\boldsymbol{w}\right) \equiv \int \boldsymbol{v}.\left(\frac{\partial \boldsymbol{w}}{\partial x_1} \times \frac{\partial \boldsymbol{w}}{\partial x_2}\right) d\Omega, \tag{31}$$

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

$$V \equiv \left\{ \boldsymbol{v} \in \left(H^1\left(\Omega\right)\right)^2 : \boldsymbol{v} = 0 \text{ on } \Gamma \right\}. \tag{32}$$

The finite element method is applied to obtain an approximation $\boldsymbol{u}_h$ to $\boldsymbol{u}$ the solution of (29) 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

$$a_1\left(\boldsymbol{u}_h;\boldsymbol{v}_h\right) - P_j a_2\left(\boldsymbol{u}_h;\boldsymbol{v}_h\right) = 0 \quad \forall \boldsymbol{v}_h \in V^h, \tag{33}$$

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 (29), 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 $\boldsymbol{e}_h = \boldsymbol{u} - \boldsymbol{u}_h$,

$$J(\boldsymbol{u}) - J(\boldsymbol{u}_h) = \int_0^1 J'(\boldsymbol{u}_h + s\boldsymbol{e}_h;\boldsymbol{e}_h)\, ds \tag{34}$$

and

$$\begin{aligned} -a(\boldsymbol{u}_h;\boldsymbol{z}) &= a(\boldsymbol{u};\boldsymbol{z}) - a(\boldsymbol{u}_h;\boldsymbol{z}) \\ &= \int_0^1 a'(\boldsymbol{u}_h + s\boldsymbol{e}_h;\boldsymbol{e}_h,\boldsymbol{z})\, ds. \end{aligned} \tag{35}$$

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

$$\int_0^1 a'(\boldsymbol{u}_h + s\boldsymbol{e}_h;\boldsymbol{v}_h,\boldsymbol{z})\, ds = \int_0^1 J'(\boldsymbol{u}_h + s\boldsymbol{e}_h;\boldsymbol{v}_h)\, ds \quad \forall \boldsymbol{v}_h \in V^h, \tag{36}$$

then we have a representation of the error as

$$J(\boldsymbol{u}) - J(\boldsymbol{u}_h) = -a(\boldsymbol{u}_h;\boldsymbol{z}). \tag{37}$$

But $\boldsymbol{z}$ depends on $\boldsymbol{u}$ so that (36) 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

$$a'(\boldsymbol{u}_h;\boldsymbol{v}_h,\hat{\boldsymbol{z}}) = J'(\boldsymbol{u}_h;\boldsymbol{v}_h), \quad \forall \boldsymbol{v}_h \in \tilde{V}^h, \tag{38}$$

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

$$J(\boldsymbol{u}) - J(\boldsymbol{u}_h) \approx -a(\boldsymbol{u}_h,\hat{\boldsymbol{z}}). \tag{39}$$

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 (29) 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 (27). 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

$$A(\boldsymbol{U};\boldsymbol{v}) = 0 \quad \forall v \in V, \tag{40}$$

where the semilinear form $A(\,.\,;\,.\,)$ contains the $a_1(\,.\,;\,.\,)$ and $a_2(\,.\,;\,.\,)$ of (29) and the inertia terms. The dual approximating problem corresponding to (38) is now

$$A'(\boldsymbol{u}_h;\boldsymbol{v}_h,\hat{\boldsymbol{z}}) = J'(\boldsymbol{u}_h;\boldsymbol{v}_h) \quad \forall \boldsymbol{v}_h \in \tilde{V}^h, \tag{41}$$

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], where the technique has been applied to the free inflation under pressure loading of a circular thin sheet clamped at its boundary with the assumption of axi-symmetry. In [4] first the deformation for a quasi-static problem is calculated for various loadings and results for this are presented together with error estimates for the finite element approximations to various quantities of interest. This is the verification. Proceeding to the fine/coarse context, taking a dynamic model with inertia terms as the fine problem and the quasi-static model as the coarse problem, error estimates for the approximation to several quantities of interest are obtained. Even though these last estimates also contain discretisation errors, they give indications of the modelling errors inherent between the coarse and fine models. This is the validation, and together verification and validation contribute to the assessment of reliability. The results of [4] demonstrate that the method is robust for this free inflation problem under the given conditions.

We have of course made no mention of the accuracy of the data of the problem; another important contributor to reliability.

5. Thermoforming Processes for Thin Polymer Sheets

Thermoforming is the process whereby thin walled structures are produced from thin sheets. In the process the sheet is heated, clamped around its boundary and inflated under pressure into or onto a (cold) mould, thus taking the shape of the mould, and then cooled. The process has two stages; the first is the free inflation as in Section 4 prior to contact with the mould, the second is inflation after part of the sheet has made contact with the mould.

Work on the computational modelling for both phases of the thermoforming process for thin polymer sheets was undertaken by de-Lorenzi and his co-workers in the 1980s/1990s, see [14], [15], who used membrane models with elastic constitutive equations and finite element discretisation techniques. Clearly these models made assumptions on the form of the deformation. Warby and Whiteman [16], [17] and co-workers extended the techniques to test these assumptions on the deformation, including elasto-plastic and viscoelastic effects and various contact conditions between the sheets and the moulds, whilst predominantly retaining the membranes models. Numerical results for the combined simulation of both phases can be found in [16] and [17].

All the simulations described above have been undertaken for sheets of oil-based polymers. Manufacturers of thin-walled thermoformed structures, particularly in the food container industry, are increasingly turning to the use of bioplastics because of their biodegrading properties which lead overall to lower long term waste. Much less is known of the properties of these biopolymers than those of the traditional oil based polymers. A first attempt at the computational modelling of thermoforming processes was made by Szegda et.al [17] for thermoplastic starch, involving various deformation models and comparing the results obtained with these.

6. Comments

The purpose of this review has been to consider the estimation of error in quantities of interest for various problems of solid deformation approximated using finite element methods. Machinery, based on the use of dual formulations, has been described for treating both discretisation and modelling errors. Our initial attempt to apply this to the problem of free inflation of thin sheets, and hence to part of the process of thermoforming has also been presented.

We seek constantly to obtain well founded models and approximations in the context of (real) thermoforming processes. These demand that assumptions are made on effects in the processes which can only be justified experimentally. We feel that the interplay between theoretical error analysis and practical computation is an important contributor to the understanding of the behaviour of the approximations and of the processes themselves.

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