Computers and Structures 185 (2017) 47–58

Contents lists available at ScienceDirect

Computers and Structures

journal homepage: www.elsevier.com/locate/compstruc

WYPiWYG hyperelasticity without inversion formula: Application to passive ventricular myocardium

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ARTICLE INFO

Article history:
Received 20 December 2016
Accepted 2 March 2017
Available online 14 March 2017

Keywords:
Hyperelasticity
Soft materials
Myocardium
Biological tissues
Splines

ABSTRACT

WYPiWYG hyperelasticity is a family of computational procedures for determining the stored energy density of soft materials. Instead of assuming the global analytical shape of these functions (the model), they are computed solving numerically the differential equations of a complete set of experimental tests that uniquely define the material behavior. WYPiWYG hyperelasticity traditionally uses an inversion formula to solve the differential equations, which limits the possible types of tests employed in the procedure. In this work we introduce a new method that does not need an inversion formula and that can be used with any type of tests. We apply the new procedure to determine the stored energy function of passive ventricular myocardium from five experimental simple shear tests.

1. Introduction

Finite element analysis is a widely known, powerful numerical method employed to solve numerically general boundary value problems [1]. Since its development in the mid-20th Century, it has replaced many analytical methods, often based on *assumed shapes* of the solution to the problem. Finite elements, as other modern numerical methods, do not assume the shape of the overall solution, but compute it using pre-defined *local interpolations* between nodal solutions.

Rubber-like materials [2] and soft biological tissues [3], frequently analyzed with finite elements [1], present a highly nonlinear behavior often considered as hyperelastic [4]. Hyperelastic behavior assumes the existence of a stored energy function such that no dissipation occurs during cyclic loading. The stored energy function cannot be measured and the analytical solution obtained directly from the measured stress-strain behavior needs some integrability conditions difficult to fulfill. The typical solution to determine the stored energy is not different in essence to many other semi-inverse methods employed to solve boundary value problems before the finite elements era. As in the Rayleigh method in structures, the classical hyperelastic model simply consists in the assumption of a possible analytical stored energy function, leaving free some material parameters. These parameters are then obtained as to best-fit the measured stress-strain behavior [9]. In essence, the parameters represent the closest solution to the actual stored energy in the predefined reduced space of global solutions, or at least they represent its effects on the available tests. The procedure to obtain these parameters is often not straightforward, and an extensive variety of optimization algorithms is employed. Remarkably, the solution obtained is not unique because the problem may not have a unique minimum [6]. The different non-unique material parameter solutions may result in very different finite element predictions in general boundary value problems, as largely reported in the literature [10–12]. We remark that the actual reason for this lack of confidence in finite element solutions is the use of an insufficient number and variety of tests to properly define the material behavior under the general loading condition that may be found at integration points during finite element simulations [6,5]. If a complete set of tests is employed, it is expected that the obtained numerical solutions are similar in these circumstances [6,13], at least under moderately large strains.

What-You-Prescribe-Is-What-You-Get (WYPiWYG) hyperelasticity is a different, purely numerical approach, to the problem of determining the stored energy function of a hyperelastic material that exactly replicates a complete set of experimental data presented to the model. It is, in some sense, similar to finite elements in solving a general boundary value problem. The WYPiWYG approach does not specify the global shapes of the stored energy terms, but computes them numerically. It does not employ material parameters. The solution is unique, explicit, without the need of any optimization procedure. Furthermore, it may be exact to machine precision if desired. The basic idea is to compute the solution of the stored energy by means of *local* shape functions, which

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http://dx.doi.org/10.1016/j.compstruc.2017.03.001
0045-7949/

interpolate numerical (nodal) values of the derivative of the stored energy terms. The computation of these nodal values is the purpose of the numerical procedure. Of course, once the stored energy is obtained, it may be employed with confidence in predictions of other boundary conditions employing finite elements as if the stored energy was an analytical single continuous function because, in short, it is an analytical piecewise function with the required smoothness. In fact, we have shown in Ref. [13] that for the isotropic case, if the procedures are fed with "experimental" data (i.e. stress-strain curves) from an analytical model fulfilling the Valanis-Landel decomposition, the ulterior WYPiWYG predictions under arbitrary loadings are equal to those obtained by the analytical model. In essence, we have numerically solved the differential equations of the experiments to obtain the true solution in piecewise form. Both the results for nonhomogeneous problems and the equilibrium iterations are the same. The computational cost is also comparable.

The WYPiWYG formulations have been developed from the ideas given in the model of Sussman and Bathe [14], which is the first WYPiWYG model. The Sussman and Bathe model for isotropic incompressible hyperelasticity employs piecewise cubic interpolation functions. In order to obtain the nodal values, they used the Kearsley and Zapas (KZ) inversion formula [15]. This formula is the analytical solution to the stored energy derivative for materials fulfilling the Valanis-Landel decomposition [16]. The KZ formula is a convergent series. Usually 20–50 terms are needed to reach the machine precision at the nodes. Between nodes the accuracy depends obviously on the number of nodes, but cubic splines require few nodes to reach indistinguishable solutions. In previous works we have extended the computational procedure to account for transverse isotropic [17] and orthotropic [18] incompressible materials using a Valanis-Landel-type decomposition equivalent to the one employed under infinitesimal deformations. In these works it was necessary to develop a more general inversion formula to solve the differential equations. In [13] we extended the procedure for compressible materials and we have shown that it is in fact a natural, equation-by-equation, extension of an infinitesimal framework accounting for bilinear behavior (with possible different moduli in tension and compression). The method can be considered as "model-free", "data-based" hyperelasticity.

One of the important features of WYPiWYG hyperelasticity, in contrast to many popular models, is that it recovers the full linear theory even in the orthotropic case. Obviously it is desirable that for infinitesimal deformations, the infinitesimal theory is recovered [21–23] and also desirable that this happens at any strain level, because every incremental (infinitesimal) deformation, even at large strains, can be considered as an infinitesimal case over a deformed configuration. From a practical point of view this also implies that engineering judgment inherited from the infinitesimal theory may be employed in the analysis of large strain models. For example, missing experimental data needed to uniquely define the material behavior may be assumed based on that experience, as for example Poisson ratios [5] (see also [24]). Experimental evidence has proved the adequacy of these hypotheses [25].

The predictive capabilities of the WYPiWYG method are excellent. It has been shown that it is capable of predicting the behavior of a large variety of materials to high accuracy; arteries in [5], superficial fascia in [20], skin in [19], incompressible rubber in [6] and compressible polyurethane foam in [13]. We will show also below excellent predictions for the passive myocardium experiments of Dokos et al. [26]. The models have been implemented in finite element codes (Dulcinea and Adina) and tested for nonhomogeneous deformations in some of these works.

One of the major difficulties in WYPiWYG hyperelasticity is that, in most practical cases, we need to solve the differential equations of the experiments by means of an inversion formula, but this is not always possible. Then, the procedure lacks a desired generality. The purpose of this paper is to generalize the WYPiWYG procedure as to bypass the need of an inversion formula, or any other add-hoc solution, and bring a procedure of more general applicability. With the new procedure proposed herein, the differential equations from any complete set of tests, uniquely defining the material behavior, can be solved numerically, obtaining therefore an also unique stored energy density in the proposed uncoupled form that "exactly" (to any desired precision) predicts the experimentally observed stress-strain behavior.

In the next section we briefly review the piecewise spline interpolation equations and recast the interpolation in a new convenient form for our purpose. Thereafter we explain the new, yet simple computational procedure. Finally we use that procedure to predict the experimental results on passive myocardium from Dokos et al. [26]. We also note that the set of tests in Dokos et al. [26] is incomplete because there are infinite stored energies even in uncoupled form, and compatible with the infinitesimal theory, that exactly predict the measured stress-strain behavior in such tests. Therefore, for our purpose, we complete the set of tests with reasonable assumptions to obtain a unique stored energy solution which preserves all independent deformation modes of the infinitesimal theory, and which can be further used with confidence in finite element predictions.

2. Piecewise spline functions in matrix form

Although different interpolation functions are possible, and may be more adequate in some cases, the piecewise cubic splines have some desirable properties of continuity and the determination is quite simple, see Refs. [17,18] for uniform and non-uniform spaced data sets, respectively. For the matter of notation simplicity, and without loss of generality of the procedure explained, we address herein the case with uniform spacing.

Assume that we have a set of known points $\{x_i, y_i\}$, $i = 1, \ldots, N+1$, that are to be interpolated by means of cubic polynomials forced to fulfill some smoothness conditions. It is convenient to normalize each subdomain $[x_i, x_{i+1}]$ defining a new normalized variable within that subdomain

$$\xi_i(x) = \frac{x - x_i}{x_{i+1} - x_i} \in [0,1] \tag{1}$$

Then, each polynomial $p_i(\xi_i(x))$, $i = 1, \ldots, N$, is defined in the unit-length $i-th$ subinterval as

$$p_i(\xi_i) = a_i + b_i\xi_i + c_i\xi_i^2 + d_i\xi_i^3 \text{ with } 0 \leqslant \xi_i \leqslant 1 \text{ and } i = 1, \ldots, N \tag{2}$$

where N is the number of intervals. For each subdomain $y_i = p_i(\xi = 0)$ and $y_{i+1} = p_i(\xi = 1)$. Between the current interval and the previous and subsequent ones, continuity of the first and second derivatives, which we denote by Y_i and Y_i' respectively, is also enforced; mathematically—note the abuse of notation in $p_i(x) = p_i(\xi(x)) = p_i(\xi)$

$$\begin{cases} p_{i-1}'(\xi_i = 1) = p_i'(\xi_i = 0) =: Y_i \\ p_{i-1}''(\xi_i = 1) = p_i''(\xi_i = 0) =: Y_i' \end{cases} \tag{3}$$

where the accent $(\cdot)'$ implies derivative with respect to the basic variable x, i.e. $p_i' = (dp_i/d\xi_i)/h$. However, we note that in the case herein addressed for simplicity all intervals have the same length, so $h := (x_{i+1} - x_i) = (x_i - x_{i-1})$, which cancels out in the previous equations. It is straightforward to obtain the coefficients of the polynomials as a function of y_i and Y_i from Eqs. (2) and (3)$_1$