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Research Paper

A general framework for application of prestrain to computational models of biological materials

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ABSTRACT

It is often important to include prestress in computational models of biological tissues. The prestress can represent residual stresses (stresses that exist after the tissue is excised from the body) or *in situ* stresses (stresses that exist *in vivo*, in the absence of loading). A prestressed reference configuration may also be needed when modeling the reference geometry of biological tissues *in vivo*. This research developed a general framework for representing prestress in finite element models of biological materials. It is assumed that the material is elastic, allowing the prestress to be represented via a prestrain. For prestrain fields that are not compatible with the reference geometry, the computational framework provides an iterative algorithm for updating the prestrain until equilibrium is satisfied. The iterative framework allows for enforcement of two different constraints: elimination of distortion in order to address the incompatibility issue, and enforcing a specified *in situ* fiber strain field while allowing for distortion. The framework was implemented as a plugin in FEBio (www.febio.org), making it easy to maintain the software and to extend the framework if needed. Several examples illustrate the application and effectiveness of the approach, including the application of *in situ* strains to ligaments in the Open Knee model (simtk.org/home/openknee). A novel method for recovering the stress-free configuration from the prestrain deformation gradient is also presented. This general purpose theoretical and computational framework for applying prestrain will allow analysts to overcome the challenges in modeling this important aspect of biological tissue mechanics.

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1. Introduction

Experimental observations show that connective tissues such as ligaments, tendons and skeletal muscle retract when excised from the body. This retraction is due to *in situ* strain–strain that exists *in vivo* in the absence of loading in the *reference configuration*. The strain and associated stress is relieved when the tissue is removed from the body, yielding a relatively *stress-free configuration*. *In situ* strains for ligaments in diarthrodial joints are in the range of 3–10% (Gardiner et al., 2001; Woo et al., 1990) and it has been shown that they contribute to the stability of joints (Ellis et al., 2006; Lujan et al., 2007). *Residual strain* (i.e. strain that exists in the tissue after it is excised from the body) is observed in many tissues such as arteries (Chuong and Fung, 1986), mitral leaflets (Rausch and Kuhl, 2013) and myocardium (Guccione et al., 1991; Omens and Fung, 1990; Wang et al., 2014). Often, geometries of biologically tissues are acquired *in vivo* and consequently the reference configuration cannot be assumed stress-free. All these various forms of prestrain, i.e. strain that exists in the reference configuration of the body of interest, can contribute significantly to the mechanical response of the system. Inclusion of prestrain is often necessary in computational models of biological tissues to obtain reasonable predictions of tissue mechanics.

One class of previously reported methods for accommodating prestrain in finite element modeling can be described as deforming a stress-free configuration to induce stress in a desired/known reference configuration. For example, in Balzani et al. (2006) this is accomplished by closing the geometry representing a radially cut artery, using a special type of spring element. In Rausch and Kuhl (2013), a stress-free configuration of mitral leaflets is stretched to conform to the *in vivo* reference configuration. In this case, the deformation map from stress-free to prestressed reference configuration was assumed to be known. This class of methods requires a sequence of forward analyses and can be executed with any finite element analysis software. The drawback is that they rely on the existence and knowledge of a stress-free configuration. In practice however, obtaining a stress-free configuration can be challenging, and there is no guarantee that it exists. For instance, in the case of arteries, the opening angle experiment was once believed to relieve the residual stress (Fung and Liu, 1989). However, it was later shown that a single cut does not relieve all the residual stress (Greenwald et al., 1997; Vossoughi et al., 1993).

In another class of methods, prestress is accounted for directly in the reference configuration without the requirement that a stress-free state exists or is known *a priori*. These methods are especially useful in the context of patient- and subject-specific modeling, since in these cases finite element models are often constructed based on image data acquired in the reference configuration. Usually the materials are assumed to be elastic and the prestress is then defined via a prestrain. The methods in this class primarily differ from each other in the definition of the prestrain. In Alastrue et al. (2007), the deformation gradient is taken from an analytical solution for the bending of a cylinder. In Weiss et al. (2005) and Dhaher et al. (2010), the deformation gradient was obtained indirectly from experimental data. In Gee et al. (2010) and later in Weisbecker et al. (2014) and Grytz and Downs (2013), the prestrain deformation gradient was obtained by solving an inverse finite element problem: given the *in vivo* reference configuration and the *in-vivo* loads, find the deformation gradient that generates the stresses in the reference configuration required to balance the applied loads. This approach requires an iterative solution due to the nonlinearity of large deformation elasticity. The method by Bols et al. (2013) is also similar in that regard, except that it attempts to recover the stress-free configuration. In general, biological tissues can have residual stresses in addition to prestress, and the methods mentioned above can be used to accommodate all forms of prestrain in a single analysis. For instance in Pierce et al. (2015) the general prestressing algorithm by Weisbecker et al. (2014) is used to account for both the residual stress and the prestress in the reference configuration of an artery. A shortcoming of the methods that start from a prestrain deformation gradient is that it cannot always be guaranteed that the induced prestress is in equilibrium with the given reference configuration. Thus, it must be verified that the applied prestrain results in equilibrated stresses. Ideally, a method to compensate for any incompatibility should be available.

The objective of this study was to develop and implement a general purpose computational framework for modeling prestrain in finite element models of biological tissues. The framework uses a prestrain gradient approach that does not require the knowledge or computability of a stress-free reference configuration. The manuscript details the theoretical foundation as well as the computational aspects of the framework. We demonstrate that previously reported methods for applying prestrain can be recovered as special cases of the framework. We also describe a method for recovering prestrain from sparse experimental data, and a method for recovering the global stress-free state from its deformation gradient. Examples illustrate the application of the framework to several test problems, including the application of prestrain to a finite element model of the knee from the Open Knee project (Erdemir, 2013, 2015; Erdemir and Sibole, 2010). The framework was implemented in the freely available finite element software FEBio (Maas et al., 2012) and can be used with any of the elastic constitutive models in FEBio.

2. Methods

2.1. Theoretical background

Consider a body in its prestressed reference configuration that is subjected to applied loading and subsequently deforms into a loaded configuration (Fig. 1). The deformation map $\boldsymbol{\varphi}(\mathbf{X})$, which maps the material coordinates $\mathbf{X}$ to the corresponding spatial coordinates $\mathbf{x} = \boldsymbol{\varphi}(\mathbf{X})$, has a deformation gradient $\mathbf{F} = \nabla_0 \boldsymbol{\varphi}$. It is assumed that for each material point, a local stress-free virtual configuration can be found in the sense of Johnson and Hoger (1995). The gradient of the local mapping from the stress-free to the prestressed reference configuration is represented by $\mathbf{F}_p$, which will be referred to as the *prestrain gradient*.

The total elastic deformation gradient $\mathbf{F}_e$ is determined by the composited deformation gradient,