

Special issues on formulations for bone remodelling around prostheses. *

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Abstract

The inclusion of special laws for the mechanical behavior of the interface between bone and implants leads to a more realistic modeling of bone adaptation around prostheses. In this paper, the incorporation of contact with friction conditions on the derivation of remodeling laws was discussed for two kinds of optimal hypotheses: bone as an optimal structure and optimal bone response. Some issues related to the choice of the objective functional and to differences between the derived optimality conditions for the two mentioned approaches are finally discussed.

1 Introduction

The ability to predict bone adaptation caused by prosthetic implantation is an important tool for technological applications and particularly, for the design of orthopedic implants and screws for bone failure repair. These techniques allow the reproduction of the long-term structural behavior of the bone-implant system (Huiskes *et al.* 1992, García *et al.*, 2002). In fact, it has been shown that computational bone adaptation models are able to reproduce effects related to the resorptive phenomenon in host bone (Van Rietbergen *et al.*, 1993, Weinans *et al.*, 1993). This is a very important issue, mainly if one considers that the problem of long-term stability of orthopedic implants (e.g., the total hip) has not been satisfactorily solved yet (Cowin, 2003).

Cementless prostheses can be classified according their mechanical behavior between *press-fitted* and *bone-ingrowth*. Essentially, a press-fitted prosthesis is a loose prosthesis: a medullary cavity is made, into which a good-fitting tapered prosthesis is put. After loading, the prosthesis will be squeezed into the bone: a press fit develops. The ingrowth, or porous coated, prostheses are coated

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with small metal particles or metal fibers that provide a bed for bone ingrowth, or with a calcium-phosphate that induces bone apposition. In this way the prosthesis is supposed to become firmly attached to the bone.

In spite of the great progress associated with the design of bone implants through computational bone adaptation models, the inclusion of appropriate interface bone/implant conditions is still an open problem.

A common assumption in the simulation of bone remodelling around cementless porous-coated prostheses is that full ingrowth applies for all the coated area. Hence, bone and stem surfaces are considered perfectly bonded during all simulation process (Weinans *et al.*, 1993, 1994, Kerner *et al.*, 1999, Bagge, 1999, Pawlikowski *et al.*, 2003).

However, this assumption misrepresents both immediate and long-term postoperative realities. In the immediate postoperative situation, contact between bone and implant is scattered, and gaps up to 3 mm always exist, even after precise insertion (Noble *et al.*, 1988, Schimmel *et al.*, 1988). It takes at least 1-2 weeks to occur bone ingrowth (Spector, 1988). Consequently, during this initial stage, the prosthesis behaves like a press-fitted one.

On the other hand, clinical observations on retrieved femoral stem specimens showed bone ingrowth over only approximately 20% of the available porous-coated surface (Fernandes *et al.*, 2002) which suggests that fully bonded coated interface is never achieved.

Some models in literature take into account the first situation, considering bone and stem surfaces to be in contact with friction (Terrier *et al.*, 1997, Fernandes *et al.*, 1999b). As pointed out by Fernandes *et al.* (2002), this approach allows the characterization of a large range of situations, from the uncoated stem to the totally coated stem. However, in this way, only the early postoperative situation is described. Consequently, as the contact conditions do not change during the remodelling process, the bone ingrowth process is not correctly simulated.

Both, early and after postoperative situations, can be modeled in some extent if one allows the model to modify the contact conditions during remodelling. This approach was proposed in Fernandes *et al.* (2002), where, starting from a contact-with-friction condition over all coated surface, a criterion for adherence is included at each time step of the remodelling simulation. If, for a certain point of the coated surface, effective contact exists and bone/stem relative displacement is less than a threshold value of $50\mu\text{m}$, then ingrowth occurs and this point is considered perfectly bonded for the rest of the process (which is a limitation also pointed out by the authors).

Mathematical models for bone adaptation found in literature have different natures. A wide group of bone remodelling laws are derived from the hypothesis that bone behaves in an “optimal” way or, at least, tries to reproduce an “optimal” structure (Fernandes *et al.*, 1999, Bagge, 1999, Lekszycki, 1999, Luo and An, 1998). Thus, the problem in focus leads to formulations analogous to those of structural optimization problems with nonlinear interface conditions (e.g. contact with friction).

The problem of structural optimization including contact conditions is thoroughly analyzed in Haslinger & Neittaanmäki (1996). Minimization of compliance is treated in Rodrigues (1993) by moving boundaries different from those in contact conditions. Applications in shape optimization, considering a moving contact boundary in order to obtain a uniform contact pressure, are discussed in

Fancello et al. (1993,1994). Optimality conditions of a performance functional depend on the derivability properties of this functional. Theoretical considerations about sensitivity analysis of the unilateral contact problem with friction were addressed by Sokolowsky (1987,1988) and Sokolowsky & Zolesio (1988).

This paper discusses the inclusion of frictional contact conditions on the derivation of remodelling laws. To this end, two approaches are addressed: those based on the hypothesis of an optimal bone topology (as in Fernandes *et al.* 1999) and those based on an optimal bone response hypothesis (Lekszycki 1999).

Section 2 presents a brief revision of a possible approach for the contact problem with friction. Section 3 discusses some aspects about the inclusion of contact conditions in the derivation of bone remodelling laws while section 4 is used for final observations.

2 Contact problem. Regularized formulation

In this section we present briefly the classical model of unilateral contact with Coulomb friction. We particularly choose a regularization of the exact equations using a penalization approach for the unilateral condition and the inclusion of an elastic reversible term on the tangential displacements (or velocities). We also restrict the equations to small displacements and rotations as well as to linear material behavior just for simplicity sake.

The variational problem can be set as searching the displacement field $\mathbf{u} \in \mathcal{K}$ such that

$$a(\mathbf{u}, \mathbf{v}) - l(\mathbf{v}) - \int_{\Gamma_c} (t_N(\mathbf{u})v_N + \mathbf{t}_T(\mathbf{u}) \cdot \mathbf{v}_T) d\Gamma = 0 \quad \forall \mathbf{v} \in \mathcal{V} \quad (1)$$

The sets \mathcal{K} and \mathcal{V} define the kinematical admissible set of displacements and variations respectively. The first two terms of (1) are the bilinear form a and linear form l representing the virtual work of internal and external forces:

$$a(\mathbf{u}, \mathbf{v}) = \int_{\Omega} \mathbf{C} \nabla \mathbf{u}^s \cdot \nabla \mathbf{v}^s d\Omega, \quad l(\mathbf{v}) = \int_{\Omega} \mathbf{b} \cdot \mathbf{v} d\Omega + \int_{\Gamma_f} \mathbf{f} \cdot \mathbf{v} d\Gamma.$$

In this expression \mathbf{C} is the elasticity tensor and $\nabla \mathbf{u}^s$ is the symmetric gradient of real displacements. The body forces \mathbf{b} are applied over Ω while known traction forces \mathbf{f} are set on the portion of the boundary called Γ_f . The last term of (1) computes the virtual work of normal and tangential contact forces (t_N, \mathbf{t}_T) applied on the portion Γ_c of the boundary, also called contact boundary. The value of the contact forces depend on the displacements and velocities of points of Γ_c through a set of tribological laws. Among other possible formulations, the classical following set of equations define a unilateral contact interface condition with Coulomb friction:

$$u_n = \mathbf{u} \cdot \mathbf{n}, \quad \mathbf{u}_T = \mathbf{u} - u_n \mathbf{n}, \quad g = u_n - s \quad (2)$$

$$t_N(\mathbf{u}) = k_N \langle g(\mathbf{u}) \rangle = k_N \langle u_n - s \rangle \quad (3)$$

$$\dot{\mathbf{u}}_T = \dot{\mathbf{u}}_T^e + \dot{\mathbf{u}}_T^s \quad (4)$$

$$\dot{\mathbf{t}}_T = -k_T \dot{\mathbf{u}}_T^e = -k_T (\dot{\mathbf{u}}_T - \dot{\mathbf{u}}_T^s) \quad (5)$$

$$\dot{\mathbf{u}}_T^s = -\dot{\xi} \frac{\partial \phi}{\partial \mathbf{t}_T} \quad (6)$$

$$\phi = \|\mathbf{t}_T\| + \mu t_N \leq 0 \quad (7)$$

$$\dot{\xi} \geq 0, \quad \dot{\xi} \phi = 0 \quad (8)$$

Equation (2) defines normal and tangential displacements on the contact boundary through projections of the displacement \mathbf{u} on the boundary normal \mathbf{n} . Function g is the actual gap between two bodies in contact while s is the initial gap. A penalization-type constitutive equation for normal traction is given by equation (3) where the Heaviside operator $\langle \cdot \rangle$ takes the positive part of the argument. Tangential velocities are split in elastic and sliding components (equation (4)). Moreover, the relationship between tangential displacements and tractions follow analogous expressions to those of perfect elastoplasticity. Tangential tractions rates depend on the elastic part of the tangential velocities. The sliding velocity is given by equation (6) i.e. its proportional to the derivative of a sliding potential ϕ defined by (7) (Coulomb model). A remarkable difference with elastoplasticity is that the slipping rule is not associative, i.e., the tangential velocity depends on the derivative of the slip function ϕ with respect to the tangential traction only, disregarding the normal component.

It must be remarked that these expressions describes the contact of a deformable body with a rigid foundation. Despite of this, these conditions can be extended for the contact of two deformable bodies substituting the boundary displacements (or velocities) u_n, \mathbf{u}_T the relative displacements between boundaries $u_n^{rel}, \mathbf{u}_T^{rel}$.

An incremental version of these equations may be obtained following similar arguments to those used for the elastoplastic model: trial tangential tractions followed to a radial returning map. Considering the solution for time step i completely known, the weak equilibrium expression at time $i + 1$ is set by (e.g. Simo & Laursen, 1990):

$$a(\mathbf{u}^{i+1}, \mathbf{v}) - l^{i+1}(\mathbf{v}) - \int_{\Gamma_c} (t_N^{i+1} v_N + \mathbf{t}_T^{i+1} \cdot \mathbf{v}_T) d\Gamma = 0 \quad \forall \mathbf{v} \in \mathcal{V} \quad (9)$$

$$t_N^{i+1} = k_N g^+(\mathbf{u}^{i+1}) = k_N (u_n^{i+1} - s)^+, \quad (10)$$

$$\dot{\mathbf{u}}_T = \dot{\mathbf{u}}_T^e + \dot{\mathbf{u}}_T^s, \quad (11)$$

$$\mathbf{t}_T^{i+1} = \hat{\mathbf{t}}_T^{i+1} - k_T \Delta \xi \frac{\hat{\mathbf{t}}_T^{i+1}}{\|\hat{\mathbf{t}}_T^{i+1}\|}, \quad (12)$$

$$k_T \Delta \xi = \begin{cases} 0 & \text{if } \hat{\phi}^{i+1} \leq 0 \\ \hat{\phi}^{i+1} & \text{if } \hat{\phi}^{i+1} > 0 \end{cases}, \quad (13)$$

$$\hat{\mathbf{t}}_T^{i+1} = \mathbf{t}_T^i - k_T (\mathbf{u}_T^{i+1} - \mathbf{u}_T^i), \quad (14)$$

$$\hat{\phi}^{i+1} = \|\hat{\mathbf{t}}_T^{i+1}\| + \mu t_N^{i+1}. \quad (15)$$

A discrete version of (9) can be obtained by using conventional finite elements. Moreover, different approaches may be used to discretize the integral equations along the contact boundary. (e.g., Wriggers et al.). The most straightforward form of solving (9) is using Newton method with a tangent matrix computed by the derivative of the residual with respect to displacements. Considering that external forces are independent of displacements we write the classical expression

$$\mathbf{R}^k = \mathbf{R}(\mathbf{U}^k) = \mathbf{F}_{int} - \mathbf{F}_{ext} - \mathbf{F}_{cN} - \mathbf{F}_{cT}, \quad (16)$$

$$\mathbf{K}^k = \frac{\partial \mathbf{R}^k}{\partial \mathbf{U}} = \mathbf{K}_{int} - \mathbf{K}_N - \mathbf{K}_T. \quad (17)$$

The residual \mathbf{R}^k in (16) is composed by internal forces, external forces (produced by \mathbf{b} and \mathbf{f}) and contact forces, split in normal and tangential parts. The consistent matrices \mathbf{K}_N and \mathbf{K}_T in (17) are obtained by deriving the contact forces in (16) with respect to displacements parameters \mathbf{U} . It is worth to mention that, due to the coupling between normal and tangential tractions in the friction behavior, the consistent matrix \mathbf{K}_T is (in the present approach) not symmetric. A symmetric tangent matrix can be obtained if we disregard this coupling, what can be interpreted as solving a contact problem with prescribed friction (Duvaut-Lions problem).

It is well known that pure penalization treatment for contact condition leads to numerical ill-conditioning. To overcome this inconvenience, Augmented Lagrangian formulation is usually included for both, normal and tangential contact behavior. This inclusion, however, does not modify the regularization approach concept of equations (2-8) and we will remain with these expressions for clarity sake.

To end this section we remark that the converged tangential consistent matrix \mathbf{K}^k (i.e., the one obtained at the solution of the nonlinear problem) play an important role on the the computation of the remodelling laws discussed in the next section.

3 Bone remodelling models

In order to work with a simplified notation, let us define the topology function h to describe the material (or material properties) distribution along the bone. This function may be of scalar or vectorial nature: bone density, dimension of microstructures, elastic coefficients, etc.

As mentioned in the introduction, an appreciable amount of papers propose (or work with) bone remodelling laws based on the hypothesis of optimal behavior of bone. Recently, a bone remodelling law of this kind was derived taken into account interface conditions with a prosthesis (Fernandes *et al.*,2002). In this work the remodelling law is derived from the optimality conditions of the following problem:

$$\begin{aligned}
\min_{h_i \leq h \leq h_s} \psi(\mathbf{u}, h) &= \int_{\Omega} \mathbf{b} \cdot \mathbf{u} \, d\Omega + \int_{\Gamma} \mathbf{f} \cdot \mathbf{u} \, d\Gamma + k \int_{\Omega} \rho(h) \, d\Omega \\
&\text{subject to} \\
a_h(\mathbf{u}, \mathbf{v}) - l_h(\mathbf{v}) - \int_{\Gamma_c} (t_N(\mathbf{u})v_N + \mathbf{t}_T(\mathbf{u}) \cdot \mathbf{v}_T) \, d\Gamma &= 0 \quad \forall \mathbf{v} \in \mathcal{V}
\end{aligned} \tag{18}$$

In this proposition, the topology variable h define the dimension and orientation of a prismatic hole within a microstructure cell. The objective function is the compliance, while the limit on the available mass of bone is indirectly considered by the third term of (18). The equilibrium equations considering contact with friction are taken as constraints. To analyze this formulation we re-write it in the following general form:

$$\begin{aligned}
\min \psi(\mathbf{u}, h) &= \int_{\Omega} \mathcal{G}(\mathbf{u}, h) \, d\Omega + \int_{\Gamma} \mathcal{J}(\mathbf{u}, h) \, d\Gamma \\
&\text{subject to} \\
\int_{\Omega} V_g(h) \, d\Omega = 0, \quad V_l(h) = 0, \\
a_h(\mathbf{u}, \mathbf{v}) - l_h(\mathbf{v}) - \int_{\Gamma_c} (t_N(\mathbf{u})v_N + \mathbf{t}_T(\mathbf{u}) \cdot \mathbf{v}_T) \, d\Gamma &= 0 \quad \forall \mathbf{v} \in \mathcal{V}
\end{aligned} \tag{19}$$

Two conditions on the variable h were included, in order to represent global and local constraints. From this problem, a Lagrangian functional is constructed and used to derive optimality conditions. The Lagrangian writes

$$\begin{aligned}
\mathcal{L}(\mathbf{u}, h, \mathbf{v}, k_g, k_l) &= \int_{\Omega} \mathcal{G}(\mathbf{u}, h) \, d\Omega + \int_{\Gamma} \mathcal{J}(\mathbf{u}, h) \, d\Gamma \\
&+ a_h(\mathbf{u}, \mathbf{v}) - l_h(\mathbf{v}) - \int_{\Gamma_c} (t_N(\mathbf{u})v_N + \mathbf{t}_T(\mathbf{u}) \cdot \mathbf{v}_T) \, d\Gamma \\
&+ k_g \int_{\Omega} V_g(h) \, d\Omega + \int_{\Omega} k_l V_l(h) \, d\Omega.
\end{aligned} \tag{20}$$

The variation of Lagrangian (19) with respect to variables \mathbf{v}, k_g, k_l recovers the non-linear state equation (1) as well as local and global constraints on h . The variations of \mathcal{L} with respect to displacements \mathbf{u} and design variable h are given, respectively, by

$$\begin{aligned}
\frac{\partial}{\partial \mathbf{u}} \mathcal{L}[\delta \mathbf{u}] &= \int_{\Omega} \frac{\partial \mathcal{G}}{\partial \mathbf{u}}[\delta \mathbf{u}] \, d\Omega + \int_{\Gamma} \frac{\partial \mathcal{J}}{\partial \mathbf{u}}[\delta \mathbf{u}] \, d\Gamma \\
&+ a(\delta \mathbf{u}, \mathbf{v}) - \int_{\Gamma_c} \left(\frac{\partial t_N}{\partial \mathbf{u}}[\delta \mathbf{u}]v_N + \frac{\partial \mathbf{t}_T}{\partial \mathbf{u}}[\delta \mathbf{u}] \cdot \mathbf{v}_T \right) \, d\Gamma,
\end{aligned} \tag{21}$$

$$\begin{aligned}
\frac{\partial}{\partial h} \mathcal{L}[\delta h] &= \int_{\Omega} \frac{\partial \mathcal{G}}{\partial h}[\delta h] \, d\Omega + \int_{\Gamma} \frac{\partial \mathcal{J}}{\partial h}[\delta h] \, d\Gamma + \frac{\partial}{\partial h} a(\mathbf{u}, \mathbf{v})[\delta h] - \frac{\partial}{\partial h} l(\mathbf{v})[\delta h] \\
&+ \int_{\Omega} \left(k_g \frac{\partial V_g}{\partial h}[\delta h] + k_l \frac{\partial V_l}{\partial h}[\delta h] \right) \, d\Omega.
\end{aligned} \tag{22}$$

Condition $\frac{\partial}{\partial \mathbf{u}} \mathcal{L}[\delta \mathbf{u}] = 0$ allows the computation of the adjoint solution \mathbf{v} . Considering symmetry of the bilinear form a , we have the following (linear) variational problem:

$$a(\mathbf{v}, \delta \mathbf{u}) - \int_{\Gamma_c} \left(\frac{\partial t_N}{\partial \mathbf{u}} v_N + \frac{\partial \mathbf{t}_T}{\partial \mathbf{u}} \mathbf{v}_T \right) \cdot \delta \mathbf{u} \, d\Gamma = \int_{\Omega} \frac{\partial \mathcal{G}}{\partial \mathbf{u}}(\mathbf{u}, h)[\delta \mathbf{u}] \, d\Omega \quad (23)$$

$$+ \int_{\Gamma} \frac{\partial \mathcal{J}}{\partial \mathbf{u}}(\mathbf{u}, h)[\delta \mathbf{u}] \, d\Gamma$$

Finally, the remodelling criterion is obtained from the stationary condition of \mathcal{L} with respect to the design parameter h , (expression (22)) evaluated at solutions \mathbf{u} and \mathbf{v} . In particular, if functions \mathcal{J} and l do not depend explicitly on the design variable h , (22) becomes an integral over Ω from which we can write the following local condition:

$$\frac{\partial \mathcal{G}}{\partial h} + \frac{\partial \mathbf{C}}{\partial h} \nabla \mathbf{u}^s \cdot \nabla \mathbf{v}^s + k_g \frac{\partial V_g}{\partial h} + k_l \frac{\partial V_l}{\partial h} = 0. \quad (24)$$

This expression is finally used to define a fixed point scheme for updating the variable h .

Up to this point, some observations can be made.

It is well known that the contact problem is not differentiable with respect to design variables (rigorous mathematical treatment of this issue should be seen in Sokolowsky (1988)). In present contact approach, non differentiability comes from the non smooth boundary constitutive equations at specific points of the tribologic curve. However, if we assume that the measure of the boundary submitted to non differentiable contact conditions is null, the problem turns differentiable and the former expressions make sense. This assumption was used with success in many works considering contact conditions. (see already mentioned references). Moreover, it is worth to remark that, although a nonlinear problem must be solved to obtain the state solution \mathbf{u} , the adjoint solution is obtained through the linear problem (23). From a numerical point of view, the adjoint solution is obtained using the converged tangent matrix (17), obtained for the converged solution \mathbf{u} .

A second observation addresses the dissipative nature of friction. Frictional contact is a history dependent problem, so does its derivative with respect to parameter h . Thus, if the mechanical behavior undergoes loadings and unloading processes, the sensitivity equations must take this incremental behavior into account and the former expressions do not apply. Thus, we limit this presentation to proportional loadings.

A final observation discusses the choice of the objective function $\psi(\mathbf{u}, h)$ for the case focused here: bone remodelling. In Fernandes et al. (1999) the functional chosen is the classic compliance, i.e., the work performed by external loads $l(\mathbf{u})$. If no contact conditions are considered, this functional is equivalent to twice the strain energy $U = \frac{1}{2}a(\mathbf{u}, \mathbf{u})$. Yet, this is not the case if frictional contact conditions are included. From equilibrium equations,

$$\psi(\mathbf{u}, h) = l(\mathbf{u}) = a(\mathbf{u}, \mathbf{u}) - \int_{\Gamma_c} (t_N(\mathbf{u})u_N + \mathbf{t}_T(\mathbf{u}) \cdot \mathbf{u}_T) \, d\Gamma. \quad (25)$$

Thus, the remodelling law based on compliance derived by Fernandes *et al.* (2002) implies computing the strain energy minus the work of contact loads. Although the biological mechanisms of remodelling are not fully understood, it seems reasonable to use the same criterion independently of the particular boundary condition (the cell will not distinguish the difference!). Due to this argument we are willing to choose $\psi(\mathbf{u}, h) = a(\mathbf{u}, \mathbf{u})$ only, as in the case of linear problems (no interface conditions). Despite of this, it is worth to note that, if the problem does not present initial gap and tangential contact displacements are small, the work of contact forces may be negligible if compared with the strain energy. In this case both approaches will give almost the same numerical results.

The next discussion focuses the choice of the formulation, i.e., the appropriate optimization problem from which the adaptation law is derived. Most works choose an objective function depending on the topological variable h . Thus, the remodelling laws are conceived as a search of an optimal state of bone. This is the case of the former formulation. In a series of papers, Lekszycki (1999,1999b,1999c), propose a different point of view, in which the remodelling laws derive from the extremization of a new performance function based on the rate \dot{h} of the topology variable. In this case, the actual state $(\mathbf{u}(h), h)$ is taken as a fixed parameter. The dependence $\mathbf{u}(h)$ means that the displacement field \mathbf{u} is related to the actual topology h by the nonlinear state equation (1). For this case, the new problem including interface conditions may be written as

$$\min \bar{\psi}(\dot{\mathbf{u}}, \dot{h}; \mathbf{u}(h), h) = \int_{\Omega} \bar{\mathcal{G}}(\dot{\mathbf{u}}, \dot{h}; \mathbf{u}(h), h) d\Omega + \int_{\Gamma} \bar{\mathcal{J}}(\dot{\mathbf{u}}, \dot{h}; \mathbf{u}(h), h) d\Gamma$$

subject to

$$\int_{\Omega} \bar{V}_g(\dot{h}) d\Omega = 0, \quad \bar{V}_l(\dot{h}) = 0, \quad (26)$$

$$\begin{aligned} & \frac{\partial}{\partial h} a(\mathbf{u}, \mathbf{v})[\delta h] + a(\dot{\mathbf{u}}, \mathbf{v}) - \frac{\partial}{\partial h} l(\mathbf{v})[\delta h] \\ & - \int_{\Gamma_c} \left(\frac{\partial t_N}{\partial \mathbf{u}}[\dot{\mathbf{u}}]v_N + \frac{\partial \mathbf{t}_T}{\partial \mathbf{u}}[\dot{\mathbf{u}}] \cdot \mathbf{v}_T \right) d\Gamma = 0 \quad \forall \mathbf{v} \in \mathcal{V} \end{aligned} \quad (27)$$

In (26) we emphasize the fact that the pair $(\mathbf{u}(h), h)$ behave as fixed parameters. Comparing (26) with (19) we note that the new constraints are set upon the rate \dot{h} while the state equation is substituted by its derivative. The Lagrangian function is now written as

$$\begin{aligned} \bar{\mathcal{L}}(\dot{\mathbf{u}}, \dot{h}, k_g, k_l, \mathbf{v}; \mathbf{u}(h), h) &= \int_{\Omega} \bar{\mathcal{G}}(\dot{\mathbf{u}}, \dot{h}; \mathbf{u}(h), h) d\Omega + \int_{\Gamma} \bar{\mathcal{J}}(\dot{\mathbf{u}}, \dot{h}; \mathbf{u}(h), h) d\Gamma \\ &+ \frac{\partial}{\partial h} a(\mathbf{u}, \mathbf{v})[\dot{h}] + a(\dot{\mathbf{u}}, \mathbf{v}) - \frac{\partial}{\partial h} l(\mathbf{v})[\dot{h}] \\ &- \int_{\Gamma_c} \left(\frac{\partial t_N}{\partial \mathbf{u}}[\dot{\mathbf{u}}]v_N + \frac{\partial \mathbf{t}_T}{\partial \mathbf{u}}[\dot{\mathbf{u}}] \cdot \mathbf{v}_T \right) d\Gamma \\ &+ k_g \int_{\Omega} \bar{V}_g(\dot{h}) d\Omega + \int_{\Omega} k_l \bar{V}_l(\dot{h}) d\Omega. \end{aligned} \quad (28)$$

Once again, the stationary condition of the Lagrangian with respect to variables \mathbf{v}, k_g, k_l recovers the derivative of the state equation as well as local and

global constraints on \dot{h} . The variations of \mathcal{L} with respect to rates $\dot{\mathbf{u}}$ and \dot{h} are given, respectively, by

$$\begin{aligned} \frac{\partial}{\partial \dot{\mathbf{u}}} \bar{\mathcal{L}}[\delta \mathbf{u}] &= \int_{\Omega} \frac{\partial \bar{\mathcal{G}}}{\partial \dot{\mathbf{u}}}[\delta \mathbf{u}] \, d\Omega + \int_{\Gamma} \frac{\partial \bar{\mathcal{J}}}{\partial \dot{\mathbf{u}}}[\delta \mathbf{u}] \, d\Gamma \\ &+ a(\delta \mathbf{u}, \mathbf{v}) - \int_{\Gamma_c} \left(\frac{\partial t_N}{\partial \mathbf{u}}[\delta \mathbf{u}] v_N + \frac{\partial \mathbf{t}_T}{\partial \mathbf{u}}[\delta \mathbf{u}] \cdot \mathbf{v}_T \right) \, d\Gamma, \end{aligned} \quad (29)$$

$$\begin{aligned} \frac{\partial}{\partial \dot{h}} \bar{\mathcal{L}}[\delta h] &= \int_{\Omega} \frac{\partial \bar{\mathcal{G}}}{\partial \dot{h}}[\delta h] \, d\Omega + \int_{\Gamma} \frac{\partial \bar{\mathcal{J}}}{\partial \dot{h}}[\delta h] \, d\Gamma + \frac{\partial}{\partial h} a(\mathbf{u}, \mathbf{v})[\delta h] \\ &- \frac{\partial}{\partial h} l(\mathbf{v})[\delta h] + \int_{\Omega} \left(k_g \frac{\partial \bar{V}_g}{\partial \dot{h}}[\delta h] + k_g \frac{\partial \bar{V}_l}{\partial \dot{h}}[\delta h] \right) \, d\Omega. \end{aligned} \quad (30)$$

The stationary condition $\frac{\partial}{\partial \dot{\mathbf{u}}} \bar{\mathcal{L}}[\delta \mathbf{u}] = 0$ allows the computation of the adjoint solution \mathbf{v} through analogous equation to (23):

$$\begin{aligned} a(\mathbf{v}, \delta \mathbf{u}) - \int_{\Gamma_c} \left(\frac{\partial t_N}{\partial \mathbf{u}}^T v_N + \frac{\partial \mathbf{t}_T}{\partial \mathbf{u}}^T \mathbf{v}_T \right) \cdot \delta \mathbf{u} \, d\Gamma &= \int_{\Omega} \frac{\partial \bar{\mathcal{G}}}{\partial \dot{\mathbf{u}}}(\mathbf{u}, h)[\delta \mathbf{u}] \, d\Omega \\ &+ \int_{\Gamma} \frac{\partial \bar{\mathcal{J}}}{\partial \dot{\mathbf{u}}}(\mathbf{u}, h)[\delta \mathbf{u}] \, d\Gamma. \end{aligned} \quad (31)$$

The stationary condition of $\bar{\mathcal{L}}$ with respect to the rate \dot{h} , (expression (30)), evaluated at solutions \mathbf{u} and \mathbf{v} gives the optimal values \dot{h} . Considering a particular case in which functions $\bar{\mathcal{J}}$ and l do not depend explicitly on \dot{h} , (30) drives to a local optimality condition analogous to (24)

$$\frac{\partial \bar{\mathcal{G}}}{\partial \dot{h}} + \frac{\partial \mathbf{C}}{\partial h} \nabla \mathbf{u}^s \cdot \nabla \mathbf{v}^s + k_g \frac{\partial \bar{V}_g}{\partial \dot{h}} + k_l \frac{\partial \bar{V}_l}{\partial \dot{h}} = 0. \quad (32)$$

We must note that equations (22) and (30) are nothing but expressions used to compute the total derivative of the objective functions ψ and $\bar{\psi}$ at the actual topology distribution h . This derivative (or gradient) information is then used to define a sequence of topology distributions through fixed point strategy. Is this mathematically constructed sequence an approximate representation of the real remodelling sequence?

We understand that the hypothesis proposed by Lekszycki as an attempt of justifying not only the final ‘‘optimal’’ state (if exist) but the path to reaching it. Therefore, a question we can formulate is: in which extent conditions (24) and (32) are different?. To answer this, let us analyze each term of them. If we take the function $\bar{\mathcal{G}}$ as the rate of \mathcal{G} , we have

$$\bar{\mathcal{G}}(\dot{h}) = \frac{\partial \mathcal{G}}{\partial \dot{h}}[\dot{h}] \implies \frac{\partial \bar{\mathcal{G}}}{\partial \dot{h}}[\delta h] = \frac{\partial \mathcal{G}}{\partial h}[\delta h].$$

Thus, in this case, the first term is equal for both problems. The second term has the same expression for both conditions. However, the adjoint solution \mathbf{v} is obtained with different equations: (23) and (31) respectively. Once again, if $\bar{\mathcal{G}}$ and $\bar{\mathcal{J}}$ are the rate of \mathcal{G}, \mathcal{J} respectively, adjoint problems (23) and (31) are

identical, so does their adjoint solution \mathbf{v} . Then, as a parcel conclusion, we can say that if we assume functions $\bar{\mathcal{G}}, \bar{\mathcal{J}}$ to be the rate of \mathcal{G}, \mathcal{J} and we disregard additional constraints, both formulations lead to the same remodelling conditions. This can be understood reminding that the gradient of a functional with respect to its variable defines the direction of the functional maximum change, which is the condition of the second approach. Despite of this, second approach is conceptually different from the first and allows the inclusion of constraints on rates \dot{h} which seems to be a natural way to represent some biological behaviors.

4 Final remarks

It seems quite reasonable that interface conditions for the contact surface between bone and implant lead to a more realistic modeling of bone adaptation around prostheses.

The incorporation of contact with friction conditions on the derivation of remodeling laws was discussed for two kinds of optimal hypotheses: bone as an optimal structure and optimal bone response.

Related to the first approach, we see that a frequent chosen functional is the inner strain energy that, in the case of linear problems, is equivalent to the work of external forces. However, we remind in this paper a subtle difference between both functionals when contact conditions are included.

Frictional contact conditions were included in the second approach and local optimality conditions were obtained. As optimality conditions for both approaches present analogous expressions, their differences were discussed. It was noted that, depending on the choice of the objective functionals, both approaches may produce similar remodeling laws.

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