Numerical analysis of a diffusive strain-adaptive bone remodelling theory

J.R. Fernández, J.M. García-Aznar, R. Martínez

Abstract

In this paper, we revisit a strain-adaptive bone remodelling problem, assuming that the rate of the apparent density at a particular location is described as a local objective function and depending on a particular stimulus at that location. Normally, continuum mathematical descriptions of adaptive bone remodelling can lead to discontinuous solutions on the global apparent density distribution. To improve this numerical solution, in this work, as the main novelty, we include the diffusion of the bone remodelling into the model. The variational problem is written as a coupled system of a nonlinear variational equation for the displacement field and a parabolic elliptic variational inequality for the apparent density. An existence and uniqueness result is stated. Then, a fully discrete problem is introduced by using the finite element method to approximate the spatial variable and an Euler scheme to discretize the time derivatives. A priori error estimates are proved from which, under adequate additional regularity conditions, the linear convergence of the algorithm is deduced. Finally, some numerical simulations are presented to demonstrate the accuracy of the approximation and the behaviour of the solution.

1. Introduction

The bone remodelling is the mechanism that regulates the relationship between the morphology of bone and its internal mechanical loads, and it is based on the fact that the bone has the ability to adapt itself to the mechanical conditions to which it is exposed.

In this paper, we revisit a bone remodelling problem introduced in Weinans et al. (1992), which is based on the principle that bone remodelling is induced by a local mechanical signal which activates the regulating cells (osteoblasts and osteoclasts). The rate of change of this apparent density, given by a function \( \rho = \rho(x,t) \), is described as an objective function which depends on a particular local mechanical stimulus at point \( x \). Since this function is a remodelling objective, it is assumed that this goal is only valid for \( \rho_b \leq \rho \leq \rho_s \), where \( \rho_b \) represents the minimal bone density and \( \rho_s \) is the maximal density of cortical bone.

Under this approach, we expected to obtain a continuous apparent density distribution due to the external applied loads that bone is supporting. However, independently of the bone remodelling theory implemented, strong bone densities discontinuities have been presented. This type of numerical effect has been termed as “patchwork” (Weinans et al., 1992) or “checkerboard” pattern (Jacobs et al., 1995). Different numerical approaches have been studied to solve this numerical phenomenon (see, e.g., Jacobs et al., 1995), being the \( L^2 \)-projection, in which apparent density is extrapolated to and averaged at the nodes, the most typical technique used. Other methodologies have been used to improve the classical continuum approach used in bone remodelling (Weinans et al., 1992; Ganghoffer, 2012) and to better describe the complex microstructural and hierarchical behaviour of bone. One of the approaches of such enriched continuum theories is the Cosserat theory (Fatemi et al., 2002). Another approach is the theory of gradient elasticity that has been recently applied, for example, to simulate stress concentrations in cortical bone by means of anisotropic gradient elasticity (Gitman et al., 2010).

Bone remodelling theories are very similar to Continuum Damage Mechanics (CDM), where damage growth is normally predicted in engineering materials, with the special particularity that bone is able to repair this damage, as it was clearly demonstrated by Doblare and García (2002). In both cases, a localisation phenomenon controls the local constitutive law leading to ill-posed problems. In CDM several classes of formulations have been successfully used to solve this problem (see, for instance, Li, 2011; Lorentz and Godard, 2011). One approach is based on the introduction of gradients of the displacement (Chambon et al., 2001), strain and/or internal variable fields by means of phenomenological considerations (Li, 2011) or derived through homogenisation (see, e.g., Lorentz and Godard, 2011). Another different approach consists on a phenomenological basis, in which the diffusion of the internal variables, specifically...
the damage, is incorporated in the formulation (Campo et al., 2007; Chen, 2000).

As far as we know, there are not previous works dealing with mathematical issues of the bone remodelling model including the diffusion term. Thus, here our aim is to continue (Weinans et al., 1992; Fernández et al., 2010), providing the numerical analysis of a fully discrete algorithm using some of the ideas introduced for the study of damage problems (see, for instance, Campo et al., 2007), proving an error estimates result, establishing its linear convergence under some regularity conditions and performing some numerical simulations which demonstrate its accuracy and behaviour.

The paper is outlined as follows. In Section 2 we describe briefly the mathematical model and we derive its variational formulation. An existence and uniqueness result is stated. Then, a fully discrete scheme, based on the finite element method to approximate the spatial variable and an Euler scheme to discretize the time derivatives, is introduced in Section 3. A main error estimates result is proved from which, under suitable regularity conditions, the linear convergence of the algorithm is deduced. In Section 4, a numerical algorithm to solve the fully discrete problem is described, and a one-dimensional numerical simulation is performed to show the accuracy of the finite element approximation and some two-dimensional numerical simulations are performed to compare the behaviour of the solution.

2. Mechanical and variational problems

Let \(\Omega \subset \mathbb{R}^d\), \(d = 1, 2, 3\), be an open bounded domain and denote by \(\Gamma = \partial \Omega\) its boundary, assumed to be Lipschitz continuous and divided into two disjoint parts \(\Gamma_D\) and \(\Gamma_N\). A generic point of \(\Omega = \Omega \cup \Gamma\) is denoted by \(\mathbf{x} = (x_i)_{i=1}^d\), and, for \(\mathbf{x} \in \Gamma\), \(\mathbf{v}(\mathbf{x}) = (v_i(\mathbf{x}))_{i=1}^d\) represents the outward unit normal vector to \(\Gamma\) at point \(\mathbf{x}\). Denote by \(\partial \Omega\), \(T > 0\), the time interval of interest. Finally, assume that the body occupying the set \(\Omega\) is being acted upon by a volume force of density \(\mathbf{f}\), it is clamped on \(\Gamma_D\) and surface tractions with density \(\mathbf{g}\) act on \(\Gamma_N\). Moreover, since the bone remodelling is unknown on the boundary, according to the damage theory we assume that the flux of apparent density is zero there.

Let \(u, \sigma\) and \(\mathbf{e}\) be the displacement field, the stress field and the linearized strain tensor, respectively, where \(e(u) = (e_i(u))_{i,j=1}^d\) is given by \(e_i(u) = \frac{1}{2} (\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i})\), for \(i, j = 1, \ldots, d\).

The constitutive bone remodelling law for the stresses is written in the following form (see Weinans et al., 1992):

\[
\sigma = 2\mu(u)e(u) + \lambda(u)\text{Div}(u)\mathcal{I} \quad \text{in } \Omega \times [0, T],
\]

where \(\mathcal{I}\) denotes the identity operator in \(\mathbb{R}^d\) (the space of second order symmetric tensors on \(\mathbb{R}^d\)), \(\text{Div}\) represents the divergence operator and \(\mu\) and \(\lambda\) are Lamé’s coefficients of the material, which are assumed to depend on the apparent density of the bone denoted by \(\rho\). These coefficients are related to Young’s modulus \(E(p)\) and Poisson’s ratio \(P\) (assumed to be independent of \(\rho\)) as follows,

\[
\mu(\rho) = \frac{E(\rho)}{2(1+P)}, \quad \lambda(\rho) = \frac{PE(\rho)}{1-P},
\]

if the plane stress hypothesis is assumed, or

\[
\mu(\rho) = \frac{E(\rho)}{2(1+P)}, \quad \lambda(\rho) = \frac{PE(\rho)}{(1+P)(1-2P)},
\]

if the plane strain hypothesis is used or if the three-dimensional case is considered. Moreover, Young’s modulus depends on the apparent density through the relation \(E(\rho) = M\rho^\gamma\), where \(M\) and \(\gamma\) are positive constants which characterize the bone behaviour.

According to Weinans et al. (1992), the evolution of the apparent density function is obtained from the following parabolic partial differential equation:

\[
\dot{\rho} = B \left( \frac{\sigma(u) \cdot e(u)}{2\rho} - S_i \right) \quad \text{in } \Omega \times (0, T), \quad \rho_0 < \rho < \rho_b,
\]

where \(B\) and \(S_i\) are experimental constants, and \(\rho_0\) and \(\rho_b\) represent the minimal density and the maximal density of cortical bone, respectively.

Thus, in this work, such a remodelling objective is modified incorporating a diffusive term for the apparent density, which leads to the following time-dependent equation for the apparent density:

\[
\dot{\rho} - \kappa \Delta \rho = B \left( \frac{\sigma(u) \cdot e(u)}{2\rho} - S_i \right), \quad \rho_0 < \rho < \rho_b,
\]

where \(\kappa > 0\) is a diffusion constant. Here, we have included a diffusion term into the constitutive equation for mathematical reasons since this new model can be studied proceeding as in the damage models.

Assuming that the process is quasistatic and denoting by \(\rho_0\) the initial apparent density, the mechanical problem is written in the following form (see Weinans et al., 1992 for further details).

**Problem.** Find a displacement field \(\mathbf{u} : \Omega \times [0, T] \to \mathbb{R}^d\) and an apparent density function \(\rho : \Omega \times [0, T] \to [\rho_0, \rho_b]\) such that \(\rho(0) = \rho_0\) and,

\[
\dot{\rho} - \kappa \Delta \rho = B \left( \frac{\sigma(u) \cdot e(u)}{2\rho} - S_i \right) \quad \text{in } \Omega \times (0, T),
\]

\[
- \text{Div}\sigma = f \quad \text{in } \Omega \times (0, T),
\]

\[
\mathbf{u} = 0 \quad \text{on } \Gamma_D \times (0, T),
\]

\[
\frac{\partial \rho}{\partial n} = \nabla \rho \cdot \mathbf{v} = 0 \quad \text{on } \Gamma_N \times (0, T),
\]

\[
\sigma\mathbf{v} = \mathbf{g} \quad \text{on } \Gamma_N \times (0, T),
\]

where Lamé’s coefficients \(\lambda(\rho)\) and \(\mu(\rho)\) were previously defined and the stress field \(\sigma : \Omega \times [0, T] \to \mathbb{R}^d\) is given by

\[
\sigma = 2\mu(u)e(u) + \lambda(u)\text{Div}(u)\mathcal{I} \quad \text{in } \Omega \times [0, T].
\]

Denote by \(Y = L^2(\Omega)\), \(E = H^1(\Omega)\) and \(H = [L^2(\Omega)]^d\), and define the variational spaces \(V\) and \(Q\) as follows:

\[
V = \{ v = (v_i)_{i=1}^d \in [H^1(\Omega)]^d; \quad v = 0 \quad \text{on } \Gamma_D \},
\]

\[
Q = \{ q = (q_i)_{i,j=1}^d \in [L^2(\Omega)]^d; \quad q_j = q_{ji}, \quad 1 \leq i, j \leq d \}.
\]

We assume now the following conditions on the applied mechanical forces and the initial apparent density:

(i) The density forces have the regularity:

\[
f \in C([0, T]; [C(\Omega)]^d), \quad g \in C([0, T]; [C(\mathcal{I}\Omega)]^d).
\]

(ii) The initial apparent density \(\rho_0\) satisfies the following conditions:

\[
\rho_0 \in C(\Omega), \quad \rho_0 \leq \rho_b(\mathbf{x}) \leq \rho_b \quad \text{for all } \mathbf{x} \in \Omega.
\]

In order to simplify the writing, for every \(p \in L^\infty(\Omega)\) we define the bilinear forms \(c(\rho, .) : V \times V \to \mathbb{R}\) and \(b(\cdot, \cdot) : E \times E \to \mathbb{R}\), and the linear form \(L : V \to \mathbb{R}\) given by

\[
c(\rho, u, v) = \int_\Omega 2\mu(u)e(u) \cdot e(v) + \lambda(u)\text{Tr}(e(u))\text{Tr}(e(v))\, dx, \quad \forall u, v \in V,
\]

\[
b(\rho, \zeta) = K \int_\Omega \nabla \rho \cdot \nabla \zeta \, dx, \quad \forall \rho, \zeta \in E,
\]

\[
L(v) = \int_\Omega f \cdot v \, dx + \int_{\Gamma_0} \mathbf{g} \cdot v \, d\Gamma, \quad \forall v \in V,
\]
where $\text{Tr}$ denotes the trace operator defined as $\text{Tr}(\tau) = \sum_{i=1}^{d} \tau_{ii}$ for all $\tau = (\tau_{ij})_{1\leq i,j \leq d}$.

By using the definition of the subdifferential, the restriction $\rho_0 \leq \rho \leq \rho_0$ is incorporated into the constitutive equation \eqref{equation:1}, leading to the following parabolic subdifferential inclusion:

$$
\dot{\rho} - \kappa \Delta \rho - \Phi(\rho, \sigma, \mathbf{u}(t)) + \partial \delta_{[\rho_0, \rho_0]}(\rho) \ni 0.
$$

Here, $\partial \delta_{[\rho_0, \rho_0]}$ denotes the subdifferential of the indicator function $I_{[\rho_0, \rho_0]}$ of the interval $[\rho_0, \rho_0]$ and the function $\Phi : Y \times Q \times Q \to Y$ has the following expression:

$$
\Phi(\rho, \sigma, \mathbf{t}) = B \left( \frac{\sigma - \ell(\mathbf{t})}{2\rho} \right) - S,
$$

where the truncation operator $\ell : \mathbb{R}^d \to \mathbb{R}^d$ is given by, for a constant $L > 0$,

$$(\ell(\mathbf{t}))_i = \begin{cases} 
L & \text{if } t_i > L, \\
\tau_i & \text{if } t_i \in [-L, L], \\
-L & \text{if } t_i < -L.
\end{cases}
$$

We note that this truncation operator is needed for mathematical reasons, in order to assure a Lipschitz property on function $\Phi$. Since this problem is considered within the small displacement theory, this is reasonable from the physical point of view.

Finally, we define the convex set of admissible apparent density functions:

$$
K = \{ \xi \in \Omega, \rho_0 \leq \xi \leq \rho_0, \text{a.e. in } \Omega \}
$$

and, using Green’s formula, we obtain the variational formulation for the mechanical problem P.

**Problem VP.** Find a displacement field $\mathbf{u} : [0, T] \to V$ and an apparent density function $\rho : [0, T] \to K$ such that $\rho(0) = \rho_0$ and for a.e. $t \in (0, T)$,

$$
c(\rho(t), \mathbf{u}(t), \mathbf{v}) = L(\mathbf{v}), \quad \forall \mathbf{v} \in V,
$$

$$
(\dot{\rho}(t), \xi - \rho(t))_Y + b(\rho(t), \xi - \rho(t))_Y \geq \frac{\Phi(\rho(t), \sigma(t), \mathbf{u}(t)))}{2}, \quad \xi - \rho(t)_Y, \quad \forall \xi \in K,
$$

where the function $\Phi$ is given in \eqref{equation:9} and the stress field $\sigma(t)$ is obtained from \eqref{equation:6}.

The existence and uniqueness of solution to Problem VP can be obtained proceeding as in Kuttler and Shillor (2006), by using the theory of pseudomonotone operators introduced in Kuttler and Shillor (1999) and already applied in the study of damage problems.

**Theorem 2.1.** Let the assumptions (i)–(ii) still hold. There exists a unique solution $(\mathbf{u}, \rho)$ to Problem VP with the following regularity:

$$
\mathbf{u} \in H^1([0, T] ; V), \quad \rho \in H^1([0, T] ; Y) \cap L^2([0, T] ; E).
$$

3. Fully discrete approximations: a priori error estimates

In this section, finite element approximations of variational problem VP are introduced. First, the spatial discretization is done by using the finite element spaces $V_h^0 \subset V$. $Q_h^0 \subset Q$ and $B_h^0 \subset Y$ and the discrete convex set of admissible apparent density functions $K_h$ given by

$$
V_h^0 = \{ \hat{\mathbf{w}}^h \in C(\Omega)^d; \hat{\mathbf{w}}^h_i \in \left[ \mathcal{P}_1(T_i) \right]^d, T \in T_h^0, \hat{\mathbf{w}}^h = 0 \text{ on } \Gamma_D^0 \},
$$

$$
Q_h^0 = \{ \hat{\sigma}^h \in L^2(\Omega)^{d \times d}; \hat{\sigma}^h \in \left[ \mathcal{P}_1(T) \right]^{d \times d}, T \in T_h^0 \},
$$

$$
E_h = \{ \hat{\xi}^h \in C(\Omega); \hat{\xi}^h \in \mathcal{P}_1(T), T \in T_h^0 \},
$$

$$
K_h = \{ \hat{\xi}^h \in E_h; \rho_0 \leq \hat{\xi}^h \leq \rho_0 \text{ in } \Omega \}.
$$

Here, we assume that $\Omega$ represents a polyhedral domain, $T^h$ denotes a triangulation of $\Omega$ compatible with the partition of the boundary $\Gamma = \partial \Omega$ into $\Gamma_D$ and $\Gamma_N$, and $P_q(T)$, $q = 0, 1$, is the space of polynomials of degree less or equal to $q$ in $T$. Moreover, the spatial discretization parameter is denoted by $h > 0$.

Secondly, the time approximation is done discretizing the time derivatives by using a uniform partition of the time interval $[0, T]$, $0 = t_0 < t_1 \leq \cdots \leq t_n = T$, and denoting by $k$ the time step size, $k = T/n$. Moreover, for a continuous function $f(t)$, let $f_n = f(t_n)$, and the subscripts $h$ and $k$ over a variable will denote the approximation of that variable with respect to both time and space.

Using a hybrid combination of both backward and forward Euler schemes, the fully discrete approximation of Problem VP is derived as follows.

**Problem VP$_h^k$.** Find a discrete displacement field $\mathbf{u}_h^k = \{ \mathbf{u}_h^{nk} \}^N_{n=0} \subset V_h^0$ and a discrete apparent density function $\rho_h^k = \{ \rho_h^{nk} \}^N_{n=0} \subset K_h$ such that, for all $\mathbf{v}^h \in V_h^0$ and $\xi_h^0 \in K_h$,

$$
c(\rho_h^{nk}; \mathbf{u}_h^{nk}; \mathbf{v}^h) = L(\mathbf{v}^h), \quad n = 0, 1, \ldots, N,
$$

$$
(\rho_h^{nk} - \rho_h^{nk-1}, \xi_h^0)_Y + b(\rho_h^{nk}; \mathbf{u}_h^{nk}, \mathbf{v}^h) \geq (\Phi(\rho_h^{nk}; \sigma_h^{nk}; \mathbf{u}_h^{nk}); \xi_h^0 - \rho_h^{nk})_Y, \quad n = 1, 2, \ldots, N,
$$

where $\rho_h^{nk}$ is a suitable approximation of the initial condition $\rho_0$ and the discrete stress field $\sigma_h^{nk} = \{ \sigma_h^{nk} \}^N_{n=0} \subset E_h$ is given by

$$
\sigma_h^{nk} = 2\mu(\rho_h^{nk})\mathbf{I} + \lambda(\rho_h^{nk})\mathbf{D}(\mathbf{u}_h^{nk}), \quad n = 0, 1, \ldots, N.
$$

The existence of a unique solution to discrete problem VP$_h^k$ can be easily deduced using classical results on elliptic variational inequalities (see Glowinski, 1984).

Next, our aim is to provide a priori error estimates on the numerical errors $\left\| \mathbf{u}_h - \mathbf{u}_t \right\|_V$ and $\left\| \rho_h - \rho_h^t \right\|_Y$. Thus, we assume the following additional regularity on the continuous solution:

$$
\mathbf{u} \in C^1([0, T] ; V) \cap C([0, T]; \mathbb{W}^{1-\infty}(\Omega)^d), \quad \rho \in C^1([0, T] ; Y).
$$

First, we recall an error estimates on the displacement fields already established in Fernández et al. (2010):

$$
\left\| \mathbf{u}_h - \mathbf{u}_t \right\|_V \leq C(\left\| \mathbf{u}_t - \mathbf{u}_h \right\|_V^2 + \left\| \rho_h - \rho_h^t \right\|_Y^2), \quad \forall \mathbf{v} \in V_h^0,
$$

where, here and in what follows, $C$ denotes a generic positive constant which depends on the continuous solution but it is independent of the discretization parameters $h$ and $k$, and whose value may change from line to line.

We obtain now error estimates for the apparent density functions. First, we rewrite the discrete variational inequality \eqref{equation:17} in the following form,

$$
(\rho_h^{nk} - \rho_h^{nk-1}, \rho_h - \rho_h^{nk})_Y + b(\rho_h^{nk}, \rho_h - \rho_h^{nk})_Y 
$$

$$
\geq (\Phi(\rho_h^{nk}; \sigma_h^{nk}; \mathbf{u}_h^{nk}); \rho_h - \rho_h^{nk})_Y 
$$

for all $\xi_h^0 \in K_h$, where $\Phi(\rho, \sigma, \mathbf{u}(t))$ and $\Phi_h(\rho, \sigma_h, \mathbf{u}(t))$.

Taking now the variational inequality \eqref{equation:11} at time $t = t_n$ and subtracting the two inequalities with $\xi_h^0 = \xi_h^n \in K_h$ we have, for all $\xi_h^n \in K_h$,

$$
(\rho_h^{nk} - \rho_h^{nk-1}, \rho_h - \rho_h^{nk})_Y + b(\rho_h^{nk}, \rho_h - \rho_h^{nk})_Y
$$

$$
\leq (\Phi(\rho_h^{nk}; \sigma_h^{nk}; \mathbf{u}_h^{nk}); \rho_h - \rho_h^{nk})_Y + b(\rho_h^{nk}, \rho_h - \rho_h^{nk})_Y
$$

$$
- (\rho_h^{nk-1} - \rho_h^{nk-1}, \rho_h - \rho_h^{nk})_Y
$$
Therefore,
\[
\left( \frac{\rho_n - \rho_{n-1}}{k} - \frac{\rho_{n+1} - \rho_{n-1}}{k} \rho_n - \rho_{n+1} \right) + b(\rho_n - \rho_{n+1}, \rho_n - \rho_{n-1})
\leq \left( \phi_n - \phi_{n+1}, \phi_n - \phi_{n-1} \right) + b(\rho_n - \rho_{n+1}, \rho_n - \rho_{n-1})
\]
\[
+ \left( \frac{\rho_{n-1} - \rho_{n+1}}{k}, \rho_{n-1} - \rho_{n+1} \right)
\]
\[
+ \left( \frac{\rho_{n-1} - \rho_{n+1}}{k} \phi_n, \rho_{n-1} - \rho_{n+1} \right)
\]
\[
+ b(\rho_n - \rho_{n+1}, \rho_n - \rho_{n-1})
\]
\[
\|
\phi_j - \phi_{j+1} \|_Y \leq C \left( \| \rho_j - \rho_{j+1} \|_Y + \| \rho_j - \rho_{j-1} \|_Y + \| u_j - u_{j+1} \|_Y \right)
\]

Taking into account that
\[
\left( \frac{\rho_n - \rho_{n-1}}{k} - \frac{\rho_{n+1} - \rho_{n-1}}{k} \rho_n - \rho_{n+1} \right) \geq \frac{1}{2k} \left( \| \rho_n - \rho_{n-1} \|_Y - \| \rho_{n-1} - \rho_{n+1} \|_Y \right)
\]

and, applying several times the Cauchy's inequality
\[\|ab\| \leq \|a\| \cdot \|b\| \quad a, b \in \mathbb{R}, \quad \|a\|, \|b\| > 0,\]

it follows that
\[
\|\rho_n - \rho_{n+1}\|_Y \leq \|\rho_n - \rho_{n-1}\|_Y + \|\rho_{n-1} - \rho_{n+1}\|_Y \leq K \left( \|\phi_n - \phi_{n+1}\|_Y + \|\rho_n - \rho_{n+1}\|_Y \right)
\]

Thus, we find that
\[
\|\rho_n - \rho_{n+1}\|_Y \leq \|\rho_n - \rho_{n-1}\|_Y + \|\rho_{n-1} - \rho_{n+1}\|_Y \leq K \left( \|\phi_n - \phi_{n+1}\|_Y + \|\rho_n - \rho_{n+1}\|_Y \right)
\]

Combining now estimates (20) and (21) it follows that
\[
\|u_n - u_{n+1}\|_Y + \|\rho_n - \rho_{n+1}\|_Y \leq C \left( \|\phi_n - \phi_{n+1}\|_Y + \|\rho_n - \rho_{n+1}\|_Y \right)
\]

Table 1

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Keeping in mind the following estimate proved in Barboteu et al. (2005):
\[
\sum_{j=1}^{n} \left( \rho_j - \rho_{j-1} - (\rho_{h} - \rho_{h-1}) \right) \leq \| \rho_0 - \rho_{h} \|_Y^2
\]

and using the previous inequalities, we deduce the following estimates for the apparent density function,
\[
\|\rho_0 - \rho_{h} \|_Y^2 + \| u_0 - u_{h} \|_Y^2 \leq \| \phi_0 - \phi_{h} \|_Y^2 + \| \rho_0 - \rho_{h} \|_Y^2
\]

and, using the regularities \( u \in C^1([0,T];Y) \) and \( \rho \in C^1([0,T];Y) \) and a discrete version of Gronwall's lemma (see Barboteu et al., 2005), we obtain the following main error estimates result.
Theorem 3.1. Denote by \((u, q)\) and \((u^{hk}, q^{hk})\) the respective solutions to problems VP and VPhk. Under the additional regularity conditions \((19)\), there exists a positive constant \(C > 0\), independent of the discretization parameters \(h\) and \(k\) but depending on the continuous solution \((u, q)\) and the data of the problem, such that, for all \(\{u_h^N\}_{n=0}^N \subset V^h\) and \(\{q_h^n\}_{n=0}^N \subset K^h\),

\[
\begin{align*}
\max_{0 \leq i \leq n} \left\{ \|u_h^n - u^{hk}_n\|_V^2 + \|q_h^n - q^{hk}_n\|_V^2 \right\} + k \sum_{n=1}^N \|\rho_n - \rho_n^{hk}\|_E^2 \\
\leq C \left( k \sum_{j=1}^N \|\rho_j - \rho_j^{hk}\|_E^2 + \frac{\|q_j^{hk} - q_j\|_V^2}{k} + \|\rho_j - \rho_j^{hk}\|_V^2 \right) + k^2 + \max_{0 \leq i \leq n} \|\rho_n - \rho_n^{hk}\|_V^2 + \max_{0 \leq i \leq n} \|u_h - u_h^{hk}\|_V^2 \\
+ \|u_h - u_h^{hk}\|_V^2 + \|\rho_0 - \rho_0^{hk}\|_V^2 + \frac{1}{N} \sum_{j=1}^N \|\rho_j - \rho_j^{hk}\|_V^2 + \frac{1}{N} \sum_{j=1}^N \|\rho_j - \rho_j^{hk}\|_V^2 - (\rho_{j+1} - \rho_{j+1}^{hk}) \bigg|_{\|V\|}^2 \bigg).
\end{align*}
\]

(22)

The above error estimates are the basis for the analysis of the convergence rate of the algorithm. Under some additional regularity conditions, we obtain the linear convergence of the algorithm.

Corollary 3.2. Let the assumptions of Theorem 3.1 hold. Define the initial condition for the apparent density function as follows,

\[\rho_0^{hk} = \rho_0.\]
where $\mathcal{P}^h$ is the $Y$-projection operator onto $B^h$. Under the additional regularity conditions:

$\mathbf{u} \in L^2(0, T; [H^1(\Omega)]^d)$,

$\rho \in H^1(0, T; Y) \cap H^1(0, T; H^1(\Omega)) \cap C([0, T]; H^2(\Omega))$,

the algorithm is linearly convergent; that is, there exists a positive constant $C > 0$, independent of the discretization parameters $h$ and $k$, such that

$$
\max_{0 \leq n \leq N} \left\{ \| \mathbf{u}_n - \mathbf{u}_n^h \|_V + \| \rho_n - \rho_n^h \|_l \right\} \leq C(h + k).
$$

(23)

The proof of this linear convergence is done proceeding as in Fernández et al. (2010). Although most of the terms can be estimated in an analogous way, we need to employ the following estimates (see Carlet, 1991):

$$
\inf_{\phi \in L^2(0, T; [H^1(\Omega)]^d)} \| \phi - \delta_t \|_{H^2(\Omega)} \leq C \| \phi \|_{L^2(0, T; [H^1(\Omega)]^d)}
$$

$$
\sum_{n=1}^{N} \left\{ \| \phi_n - \phi_n^{h} \|_{H^2(\Omega)} + \| \phi_n - \phi_n^{h} \|_{L^2(\Omega)} \right\} \leq C \| \phi \|_{L^2(0, T; [H^1(\Omega)]^d)}.
$$

4. Numerical results

Next, we briefly describe the numerical resolution of Problem $VP^h$ and we show some of the numerical results obtained for a simple one-dimensional example to show the behaviour of the solution.

4.1. Numerical resolution of Problem $VP^h$

We recall that the variational spaces $V$, $Q$ and $B$ and the convex subset $K$ were approximated by the finite element spaces $V^h$, $Q^h$ and $B^h$ and the discrete convex set $K^h$ given in (12)–(15), respectively.

The discrete approximations are obtained solving the following linear variational equation,

$$
\mathbf{u}_n^h \in V^h : \ c(\rho_n^h, \mathbf{u}_n^h; \mathbf{v}) = L(\mathbf{v}) , \ \forall \mathbf{v} \in V^h. \ \ n = 0, 1, \ldots, N.
$$

It is easy to check that this problem leads to a linear system, which is solved by using classical Cholesky’s method. Here, we note that the initial discrete apparent density is known.

The discrete stress field is now updated using equation (18), and the discrete apparent density function $\rho_n^h$ is then obtained solving the following discrete variational inequality, for all $\mathbf{v}^h \in K^h$:

$$
\rho_n^h \in K^h : \ \left( \rho_n^h, \mathbf{v}^h - \rho_n^h \right)_V + kb(\mathbf{v}^h, \mathbf{v}^h - \rho_n^h) \\
\geq k \left( \Phi(\mathbf{u}_n^{h-1}, \mathbf{u}_n^{h}), \mathbf{v}^h - \rho_n^h \right)_V + \left( \Phi(\mathbf{u}_n^{h-1}, \mathbf{v}^h - \rho_n^h) \right)_V.
$$

A penalty-duality algorithm is employed for its numerical resolution.

Finally, we note that this algorithm was implemented on a Core i7 3.4 Ghz PC (with 8 Gb of RAM Memory) using MATLAB, and a typical 1D run ($h = k = 0.01$) took about 1 s of CPU time and a 2D run spent about 10 s for each iteration.

4.2. Numerical convergence in a one-dimensional example

In order to show the accuracy of the algorithm, we consider the following simple one-dimensional problem.

**Problem T1D**. Find a displacement field $u : [0, 1] \times [0, 1] \to \mathbb{R}$ and an apparent density function $\rho : [0, 1] \times [0, 1] \to [0.01, 1.74]$ such that

$$
-\frac{\partial \sigma}{\partial x}(x, t) = 0 \ \ x \in (0, 1), \ \ t \in (0, 1),
$$

$$
\rho(x, t) - \frac{\partial^2 \rho}{\partial x^2}(x, t) = \left( \frac{\sigma(x, t) q \rho(x, t)}{2 \mu(x, t)} - 0.25 \right) \ x \in [0, 1], \ \ t \in [0, 1),
$$

$$
u(0, t) = 0 \ t \in (0, 1),
$$

$$\frac{\partial \rho}{\partial x}(0, t) = \frac{\partial \rho}{\partial x}(1, t) = 0 \ t \in (0, 1),
$$

$$\sigma(1, t) = -10^4 e^t \ t \in (0, 1),
$$

$$\rho(x, 0) = 0.8 \ x \in [0, 1].
$$

We note that this problem corresponds to the mechanical problem $P$ with the following data (the area of the cross-section is $A = 1$ m$^2$):

$$
\Omega = (0, 1), \ T = 1 \text{ day}, \ E(\rho) = M \rho^2. \ M = 100 \text{ N m}^2/\text{kg}^2, \ \gamma = 2,
$$

$$\kappa = 1, \ B = 1, \ \rho_m = 0.01 \text{ kg/m}, \ \rho_s = 1.74 \text{ kg/m}. \ S_r = 0.25 \text{ kg/ms}, \ \rho_0 = 0.8 \text{ kg/m}. \ f = 0 \text{ N} , \ \ g(t) = 10^{-3} e^t \text{ N for } t \in [0, 1].
$$

This problem is solved in order to demonstrate the numerical convergence of the algorithm. We consider several uniform partitions of both the time interval and the domain, dividing $\Omega = (0, 1)$ into $n$ segments. Therefore, the spatial discretization parameter $h$ equals to $\frac{1}{n}$ and, since the exact solution cannot be calculated, we used in its place the solution obtained with $n = 2^{12}$ and $k = 10^{-6}$.

Varying the discretization parameters $h$ and $k$, in Table 1 we depict the numerical errors (multiplied by 100) given by

$$
E^h = \max_{0 \leq n \leq N} \left\{ \| \mathbf{u}_n - \mathbf{u}_n^h \|_V + \| \rho_n - \rho_n^h \|_l \right\}.
$$

Moreover, the evolution of the error depending on $h + k$ is plotted in Fig. 1. The convergence of the algorithm is clearly observed, and the linear convergence rate seems to be achieved (see Corollary 3.2).

Finally, we aim to understand the influence of the diffusion coefficient. Therefore, we consider a slight modification of Problem T1D, assuming now that $g = 0 \text{ N}$ and that $f = 5x^2 \text{ N/m}$. Using discretization parameters $h = 2^{12}$ and $k = 10^{-4}$, in Fig. 2 we plot

Fig. 3. Finite element mesh of the 2D femur simulated.
the apparent density at final time $T = 1\, s$, for different diffusion coefficients. We note that, when the diffusion coefficient is smaller, the solutions have strange oscillations near the right corner $x = 1$. This way, it seems that diffusion leads to the smoothness of the solution and the removal of such oscillations.

4.3. Numerical results for two-dimensional problems

In order to test the different behaviour of the numerical approach established by the bone remodelling using the damage diffusion, we have simulated a classical benchmark problem corresponding to one 2D femur (see Fig. 3). To simulate the actual connection between the two cortical layers, a side plate is included in ABCD linking both lateral nodes (see, for details, Fernández et al., 2010). The finite element mesh corresponding to the proximal femur has 1144 nodes and 2139 elements. We assume that the lower horizontal node is clamped (the left lower point is fixed, whereas the rest of this boundary is fixed through the vertical direction). We consider one daily loading condition due to the walking activity. This load consists on a distributed force acting on the femoral head, where its resultant is 2317 N forming $24^\circ$ with the vertical direction, and on the higher trochanter, where its resultant is 703 N oriented $28^\circ$ with respect to the vertical. Nevertheless, most of the data that define this example have been completely described in our previous work from the same authors (see, for details, Fernández et al., 2010).

The following data have been used in this simulation (see Fernández et al., 2010; Weinans et al., 1992):

\[ T = 700 \text{ days}, \quad E(\rho) = M \rho^\gamma, \quad M = 3790 \text{ MPa cm}^2/\text{g}^2, \quad \gamma = 3, \]
\[ \kappa = 10^{-9}, \quad B = 1 \text{ (g/cm}^3\text{)}^2 \text{ (MPa day)}^2, \quad \rho_a = 0.01 \text{ g/cm}^3, \]
\[ \rho_b = 1.74 \text{ g/cm}^3, \quad S_r = 0.004 \text{ J/g}, \quad \rho_0 = 0.8 \text{ g/cm}^3, \quad P = 0.3. \]

After the simulation of 700 analysis using a time increment of one day, in Figs. 4 and 5, we show the apparent density distribution obtained with our model in the integration points used in the mesh. In fact, in Fig. 4 we can see this distribution with a clear “checkerboard” pattern. However, if we include the apparent density diffusion, we can observe the distribution of the apparent density and we can see how this pattern disappears in Fig. 5, showing a smooth density distribution.

The addition of the diffusion of the apparent density not only influences on the spatial distribution of the apparent density, but also in the time convergence.

As can be seen in Fig. 6, the inclusion of the apparent density diffusion allows to accelerate the convergence, quickly achieving the equilibrium.
5. Conclusions

In this work, we have studied the effect of including the apparent density diffusion on one specific bone remodelling algorithm. The mathematical interest of this procedure has been twofold. First, the existence of a unique solution to this problem, which is an open problem yet for the non-diffusive model, has been stated by using the techniques developed for the analysis of damage.

Fig. 5. Apparent density distribution in the femur including apparent density diffusion: (a) 180, (b) 270, (c) 350 and (d) 500 days.

Fig. 6. Temporal evolution of the apparent density distribution in the femur: (a) not including and (b) including apparent density diffusion.
problems. Secondly, we have proved similarly an a priori error estimates, Theorem 3.1, improving the $L^2$ estimates of the study presented in Fernández et al. (2010), adding an energy term for the apparent density. Finally, a numerical analysis, 1D and 2D finite element based bone remodelling simulations have been presented. These results clearly show a great improvement in the numerical behaviour of the bone remodelling simulations when diffusion term is included. In fact, we have shown that bone remodelling algorithms present localisation problems that different authors have termed as “checkerboard” or “patchwork” (see Jacobs et al. (1995)). However, a possible alternative to solve this problem has been proposed in this work, although other different techniques (normally used in damage localisation, such as, enriched continuum theories) could also be used in the future to improve bone remodelling algorithms.

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