Computational simulation of idealized long bone re-alignment

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Abstract

The RFEM3D (Remodeling Finite Element Method—3-Dimensional) computer program has been modified to allow its use to simulate the gradual straightening of a long bone that has fractured and then healed with a mal-alignment. The simulations using a “signed” quantity to drive the net remodeling process—such as the axial stain—give qualitatively correct results. However, the simulations using strain energy density—always a positive quantity—are unable to simulate the coordinated simultaneous bone addition and resorption that matches the clinically observed net remodeling.

Introduction

The adaptation of bone shape to its mechanical usage has been a topic of considerable recent interest, and advances in understanding bone’s adaptation to mechanical use are expected to result in specific strategies to improve understanding and clinical treatment of specific bone disorders. One such disorder sometimes seen in bone is the mal-alignment of femoral shaft fractures that can result in an angulation from the original long axis of the bone. Over time, this angulation will gradually tend to correct itself by a functional adaptation to its mechanical usage [14, 15, 5]. The adaptation involves simultaneous and coordinated sub-processes with areas of net bone resorption and areas of net bone deposition. And, although complete correction is not generally expected, the process is observed to produce better alignment in immature bone that is still growing. Although this specific example of net surface bone remodeling is not a frequent clinical problem, it has been the subject of several “thought experiments” used to develop and validate theoretical notions of how long bones change shape in response to mechanical usage [3, 4, 5].
With the relatively recent incorporation of net bone remodeling theories into computational simulation programs based on the finite element method (e.g., [6, 7, 9]), it is now possible to computationally perform these “thought experiments” to help determine which theories are applicable to this example of gradual realignment [10, 12, 13].

The motivation for the present study was to begin to incorporate multiple net remodeling theories into one computational program, RFEM3D (Remodeling Finite Element Method—3-Dimensional) and to then investigate the similarities and differences in shape change simulations. In this initial application, the shape changes of an idealized model of an angulated bone were investigated. The simulations reported here were based on the Surface Remodeling portion of Cowin’s Adaptive Elasticity [1] and Huiskes’ Strain Energy-based adaptive theory [9].

Methods

For this study, three-dimensional finite element models—intended to represent an idealized representation of a child's femur—were developed, and the RFEM3D (Remodeling Finite Element Method—3-Dimensional) program [6, 7] was used to simulate the net remodeling activity. The RFEM3D program was modified to allow for three different surface remodeling theories to be incorporated into the program, all based on the notion that the functional adaptation is driven by the error between mechanical measures of conditions in the angulated bone as compared to the straight one [1]. Rust [12] has shown that the use of axial stain and a mechanical intensity scalar [8] both give quantitatively similar results that compare well with the clinically observed processes. However, the strain energy formulation [9]—because it lacks a "sign"—adds bone both where it should be added, but also in areas where resorption should occur. Unfortunately, although the qualitative trends were observed in the earlier study [12, 13], the computational implementation was not robust enough to allow for the major element shape changes needed to simulate substantial realignment of the bone.

Changes to RFEM3D

The RFEM3D program has been continually refined since it was originally completed in 1983. For this application, two notable changes were made in the program. The first change was made to overcome a problem associated with large element distortions that can occur in some surface remodeling simulations. The program assumes that the finite elements are always oriented so that periosteal surfaces are on the “+s” face of an element (nodes 1,2,5,6,9,13,17,18), and endosteal surfaces are on the opposite, “-s” face (nodes 3,4,7,8,11,15,19,20), see Figure 1.

Originally, the program allowed for large changes in element volumes when bone is added at either surface, but simulations of extensive bone resorption prematurely terminate program execution when the element volume reaches zero.

Because each element was assumed to be independent of other elements, the gross shape changes associated with the angulated bone problem could not be accomplished. This problem has been addressed by Oden [11]. For the present application, the use of “tied” elements was developed so that 2 or more elements could have their surface motion coordinated. The initial FEA
of the model also had a search algorithm added to identify endosteal elements and their adjacent periosteal elements. These elements were then listed as “tied” for the surface remodeling simulations, and the element face common to both elements was allowed to undergo a spatial relocation equal to the average of the endosteal and periosteal relocation. In that way, the elements move in tandem, and via this coordination, retained non-zero element volumes as long as the bone’s wall thickness remained finite.

The second change was also needed to maintain appropriate element geometries during the remodeling simulations. The program originally allowed for bone to be either resorbed or added in the normal direction to the existing bone surface. Although this is a good representation of the physiological process, it generated difficulties for these simulations. For the angulated bone model, endosteal and periosteal surfaces were no longer normal to the long axis of the bone (the z-axis). Consequently, instead of having the elements in the bone’s cortex simply get thicker or thinner, the elements also had a component that changed element “height” (length in the z-direction). The resulting element shape distortions led to singularities at nodal locations when nodal strains were calculated, terminating the simulation prematurely. Thus, version 3.7 of the program was made into a special case version—3.7b—in which the z-component of the surface shape change can be maintained at zero.

Models: Several series of finite element models were constructed for the study. Following an h-convergence test to determine the proper mesh refinement, a model with 4000 nodes and 704 of the 20-noded isoparametric 3-D hexagonal elements were used. The PATRAN (PDA Engineering, Costa Mesa, CA) program was used to generate all models. Once a template session file was created with PATRAN, changes to the session file allowed for easy changes in mesh refinement and in the degree of initial angulation.

Common for all models were the following:

Isotropic material properties: E = 18.97 GPa, v = 0.3

Geometry: Initial Inner Radius: 0.01m
Initial Outer Radius: 0.016m
Height: 0.25 m in the “Z-direction”

Boundary Conditions: Nodes fixed at base (z=0)
Loading: Four Concentrated point loads (75N each) applied at the model’s top

Equilibrium Model: To find the remodeling equilibrium strains before
imposing the initial angulation, the model was a right circular cylinder.

The initial angulation consisted of having an angle of $10^\circ$ with respect to the vertical at the base, and the same angle at the top.

![Figure 2. Finite element models and points of load application for the right circular cylinder used to idealize the initial model configuration, and the initial angulation.](image)

The cross section of the model at the mid height of the length has four points of particular interest, as indicated in Figure 3.

![Figure 3. View of the mid-height cross section showing 4 points used to characterize remodeling regions.](image)

**Remodeling Rules:**

**Axial Strain.** The first remodeling rule used was based on the suggestion by Cowin and Van Buskirk [1]. However, rather than use the full strain tensor, this simulation used only the axial stain component. Thus the first order rate equation was:
\[ U = C_3(Q)[\varepsilon_{zz}(Q) - \varepsilon_{zz}^0(Q)] \]  

(1)

where \( U \) is the “velocity” (change in position over time) of the bone’s external bone surface at point \( Q \), \( C_3(Q) \) is the remodeling rate parameter, \( \varepsilon_{zz}(Q) \) is the strain at point \( Q \), and \( \varepsilon_{zz}^0(Q) \) is the remodeling equilibrium strain at point \( Q \). Depending upon the location of the point \( Q \), and the choice of the sign, and magnitude of \( C_3 \), this equation can produce a number of net remodeling scenarios. Depending upon the sign of the strain difference, \([\varepsilon_{zz}(Q) - \varepsilon_{zz}^0(Q)]\), and the sign of \( C_3 \), the “velocity,” \( U \), calculated in equation (1) can be made positive (bone deposition) or negative (bone resorption).

Thus, it is important to note that equation (1) can give the range of potential net remodeling responses that might be expected. Just as important, however, is the need to develop some basis for choosing the constants so that a priori predictions of shape change can be made. Different values for the constants have been previously estimated from trial and error simulations of animal experiments reported in the literature [2]. In that study it was found that to make equation (1) match the experimental results, the values of \( C_3 \) depended on whether the surface point \( Q \) was an endosteal or periosteal surface. This distinction is biologically reasonable considering the nature of the different environments in the medullary canal as opposed to the periosteum. In addition, the magnitude and sign of the constants had to be adjusted based on whether point \( Q \) was accustomed to seeing tensile or compressive strains. This distinction is more questionable, but might be rationalized depending upon the nature of the “mechanicostat.” For example, if the stimulus for net remodeling is based on dilatational strain of the cells or based on the direction of fluid flow assuming a streaming potential as the transduction mechanism, then the distinction between tensile and compressive strains may be biologically reasonable.

In any case, for this idealized study, \( C_{p3} = -35 \text{ m/yr} \) and \( C_{e3} = +35 \text{ m/yr} \). Thus the constant was independent of the sign of the axial strain, and the magnitude was the same for the endosteal and periosteal surfaces, but with opposite signs. Based on the initial uniform compression for the straight cylinder and the degree of mal-alignment, points 1 and 2 shown in Figure 3 were put into tension in the mal-aligned model. For Point 1 on the periosteal surface, with \( C_3 < 0 \), there was a negative “velocity” from equation (1), so the bone at that surface resorbed. Meanwhile, for Point 2 on the endosteal surface, with \( C_3 > 0 \), there was bone deposition.

Based on the models used here, the maximum strain difference, \([\varepsilon_{zz}(Q) - \varepsilon_{zz}^0(Q)]\) was \( 1.47 \times 10^{-4} \). Based on that strain difference and the chosen values for the constants, \( C_3 \), the maximum initial velocity, \( U \), was \( 5.145 \times 10^{-3} \text{ m/year} \). The simulated time for the analysis was 1 year accomplished with 35 complete time steps. All analyses were run on the Departmental CRAY Y-MP/EL94 Model 250 computer system.

**Strain Energy.** The second remodeling rate rule used in the study was based on the suggestion by Huiskes et al. [9]. It employs a threshold mechanical stimulus that is required to start the process of net remodeling, sometimes referred to as a “lazy zone” or a “dead zone.” In addition, the mechanical stimulus is not taken to be the strain tensor or a single component, but a scalar, the strain energy density, \( U = \frac{1}{2}E_{ij}T_{ij} \).

Then the rate equation is written as:
where $X$ is the surface growth, $C_s$ is the remodeling rate coefficient, $2s$ is the width of the "lazy zone," and $U_n$ is a homeostatic strain energy density.

Two slightly different analyses were performed in the simulations. The first, termed site dependent, was based on each surface point having a unique homeostatic strain energy density, $U_n$. Each node’s homeostatic value was taken to be the strain energy calculated using the initial right circular cylindrical model. The second analysis was based on a site independent analysis where the homeostatic strain energy was assumed to be everywhere the same. The value was taken to be the average of the nodal strain energy densities in the initial straight model. The half width of the “lazy zone” was 10% of the homeostatic strain energy density, $U_n$. The remodeling rate constant, $C_s = 1. \times 10^6$ was used for both analyses and was chosen to give a similar initial velocity to the case studied with equation (1), based on differences between the strain energy, $U$, and the homeostatic strain energy densities, $U_n$.

Again, the simulated time was 1 year with 35 complete time steps. All analyses were run on the Departmental CRAY Y-MP/EL94 Model 250 computer system.

Results and Discussion

All of the analyses ran to completion, with significant net bone remodeling sites at the mid-height of the bone, as expected. Also as expected, complete re-alignment was not achieved with the remodeling rate constants that were chosen. Despite improvements in the program, the mesh has become distorted in some regions so that to achieve substantially more realignment, a re-meshing capability may be required.

The new geometries, shown in Figure 4, show that the adaptive elasticity rule used with axial strain, equation (1), was able to show the coordinated bone resorption and formation that is observed clinically. Note, however, there is a small region at the exact mid-height of the bone corresponding to point 3 in Figure 3 that has moved in the wrong direction (bone is added rather than resorbed). An examination of the axial strain distributions, shown in Figure 5, reveals the reasons.

Figure 4 Cut-away views of the shape changes calculated using the equation (1), left, and equation (2), right.
First, note that because $\varepsilon_0^0(Q) < 0$ for all points $Q$, the term $-\varepsilon_{zz}^0(Q)$ in equation (1) has a positive value. Next, consider the strains due to the imposed angulation, as shown in Figure 5. The following uses qualitative notation as follows: (++) for large magnitude tension; (+) for tension; (-) for compression; and (- -) for large magnitude compression. Point 1 (++) is in tension with a larger magnitude than the tension at Point 2 (+). Point 3 (-) is in compression, but with a magnitude less than $\varepsilon_{zz}^0(3)$, while Point 4 (- -) is in compression with a magnitude greater than the equilibrium value. Thus, combining the qualitative notation with equation (1) gives:

Point 1: $U = -C(++) < 0$; Resorption
Point 2: $U = +C(++) > 0$; Formation
Point 3: $U = +C(-+) > 0$; Formation?
Point 4: $U = -C(---) > 0$; Formation

For the region somewhat near Point 3, with compressive strain magnitudes larger than the magnitude of the compressive equilibrium value, the velocity is negative, giving resorption as expected. However, in this particular model, at the concentrated region in the immediate neighborhood of Point 3 (see Figure 5), the magnitude of the compressive strains is less than the equilibrium one, and so formation begins.

**Figure 5.** Axial strain distribution in the mal-aligned model (top), and strain energy density distribution in the mal-aligned model (bottom).
For the strain energy density based predictions, the greatest change in magnitude corresponds to point 4, as seen in Figure 5, and there is substantial bone deposition there. For the site dependent solution, the region at Point 1 has a somewhat elevated strain energy density level (above the threshold), and so bone is also added there, but much less noticeably. It is, however, significant that the strain energy density formulation, as used here, is unable to achieve the correct coordination of simultaneous bone resorption and deposition that is required.

The simulation using the site independent formulation is virtually identical, except bone is added only in the region near Point 4. Note that because the analyses reported here had a uniform axial load in the initial straight configuration, the difference between the site dependent and the site independent cases was minimal.

Conclusions

The simple idealized example analyzed here has served several purposes. Perhaps most significant, it highlights the inability of the strain energy density formulation to realistically simulate the expected net surface remodeling behavior of the mis-alignment problem. And, although the axial strain simulation also had some anomalous regions of bone deposition, it qualitatively achieved most of the expected results.

Finally, of course, the problem of net bone remodeling is much more complex than addressed here. For example, experimental evidence is mounting that spatial and/or temporal gradients of the mechanical measures are of key importance. Neither is addressed here. Furthermore, the need for more sophisticated modeling of the biology is clearly evident. However, with the modest methodological improvements to the RFEM3D program reported here—accommodating a greater degree of mesh distortion and multiple remodeling rate theories—the interest and motivation for developing more robust and versatile computational vehicles for testing and understanding the fundamental mystery of how biological structures respond to their mechanical environment is even more compelling.

References


**Acknowledgments**

The research has been supported, in part, by grants from the NIH (AR40655), the Pittsburgh Supercomputing Center (MSM8600007), and the Louisiana Education Quality Support Fund (ENG/B29).