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Stochastic multiscale modeling of elastic properties of bone ultrastructure

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1. Introduction

Amazing mechanical properties of bone, coupling stiffness, strength and lightweight, are due to its complex hierarchical structure spanning several length scales, from the organ to the molecules. Bone hierarchical structure results from a lifelong reorganization of bone material known as bone remodeling. Abnormal remodeling related to bone diseases such as osteoporosis can lead to lower bone quality and increased risk of fracture. Thus, analysis of bone microstructure and mechanical properties can help detecting early signs of bone diseases. Biomechanical modeling and numerical simulations represent a fast and powerful tool to analyze bone quality based on clinical data such as porosity and degree of mineralization. However, their clinical application is limited by the lack of patient-specific data on bone microstructure which can be hardly inspected by commonly used *in vivo* experimental techniques. In this paper, we present an original approach aiming at getting around this difficulty by combining multiscale modeling and stochastic representation of modeling variables. In particular, this latter will allow accounting for the incomplete knowledge of patient-specific data on bone microstructure while preserving robustness of modeling and reliability of numerical results.

2. Methods

Multiscale modeling: Continuum micromechanics. Continuum micromechanics theory [Suquet, 1997] is used to obtain a multiscale description of bone tissue as previously described in [Sansalone *et al*, 2010, 2012]. For sake of simplicity, only three scales will be considered (see Figure 1). The solid matrix of bone tissue (characteristic length: 10^{-3} m) is referred to as ultrastructure. Zooming in, ultrastructure is seen as an assembly of elongated collagen molecules embedded in mineral foam (characteristic length: 10^{-5} m). At a deeper observation (characteristic length: 10^{-7} m), the mineral foam is described as a highly disordered mixture of mineral and adsorbed water (filling the intercrystalline spaces). Thus, two homogenization steps are required to compute the effective properties of bone ultrastructure. First, the effective

elastic properties of the mineral foam will be computed as a mixture of mineral and water (step I, Self-Consistent approximation). Then, the effective elastic properties of the ultrastructure will be computed considering collagen inclusions in the mineral foam (step II, Mori-Tanaka approximation).

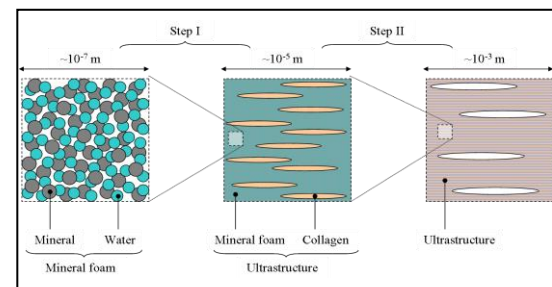


Figure 1 Three-scale model of bone ultrastructure.

Stochastic modeling: MaxEnt principle.

Uncertainties about actual values of the modeling variables motivate the use of either a parametric or a stochastic approach to describe their variations. Modeling variables can be considered as either free parameters (f.p.) or random variables (r.v.). These latter require to build suitable distribution functions. We constructed the probability laws of the uncertain parameters of the model using the Maximum Entropy (MaxEnt) principle [Jaynes 1957a, 1957b]. In the context of the information theory, a measure of the uncertainty for probability distributions has been introduced in [Shannon, 1948]. The MaxEnt principle consists in maximizing this entropy subjected to constraints defined by the available information. The MaxEnt principle was used to build stochastic mechanical models by [Soize, 2001]. Following this approach, we developed suitable probability laws for the elastic coefficients of bone constituents, namely the Young modulus and Poisson coefficient of collagen (Y_{col} , V_{col}) and mineral (Y_{HA} , V_{HA}) and the bulk modulus of water (K_w). The other modeling variables were considered as f.p.s. The available information for each r.v. X was assumed to be its range $[X_{min}, X_{max}]$, mean μ_X and dispersion δ_X . More details on the resulting probability distributions can be found in [Guilleminot and Soize, 2013].

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Coupling Multiscale and Stochastic modeling

The first homogenization step requires computing the elasticity tensor of the mineral foam (\mathbf{C}_{foam}) based on the volume fractions of mineral and water in the foam (f.p.s $f_{\text{HA,foam}}$ and $f_{\text{w,foam}}$, respectively) and their elastic properties (input r.v.s Y_{HA} , V_{HA} , and K_{w}). Both mineral and water particles were assumed to have spherical shape (Figure 1, on the left). The resulting mixture is isotropic. Therefore, \mathbf{C}_{foam} can be parameterized by the Young modulus Y_{foam} and Poisson coefficient V_{foam} . The second step requires computing the elasticity tensor of the ultrastructure ($\mathbf{C}_{\text{ultra}}$) based on the volume fractions of collagen and mineral foam in the ultrastructure (f.p.s $f_{\text{col,ultra}}$ and $f_{\text{foam,ultra}}$, respectively) and their elastic properties (input r.v.s Y_{col} and V_{col} and output r.v.s Y_{foam} and V_{foam}). Collagen was assumed to have cylindrical shape (Figure 1, in the middle). The resulting mixture is transversely isotropic. Coefficients of \mathbf{C}_{foam} and $\mathbf{C}_{\text{ultra}}$ are output r.v.s whose distributions depend on the probability laws of the input r.v.s Y_{col} , V_{col} , Y_{HA} , V_{HA} , and K_{w} .

3. Results and Discussion

Large-scale numerical simulations were performed by letting each f.p. span its physiological range of values and each input r.v. vary according to its probability distribution. Input r.v.s were sampled using a Monte Carlo method and an *ad hoc* generator of statistical independent realizations. The number N of realizations was chosen so as to ensure convergence of the realizations of the input r.v.s to their probability distributions. Thus, each run of the numerical model corresponds to a given set of values of the f.p.s and to a specific realization of the input r.v.s. For each run, the elastic tensor of the bone ultrastructure was computed using the multiscale procedure described above. Then, for each set of values of the f.p.s, we ended up with N estimates of \mathbf{C}_{foam} and $\mathbf{C}_{\text{ultra}}$. Numerical simulations were run using values of f.p.s and r.v.s typical for cortical bone. In Fig. 2, the running mean (on the top) and dispersion (on the bottom) of the axial modulus of bone ultrastructure in the direction of the osteonal axis ($Y_{\text{ultra},3}$) are shown. These results are obtained using values of mineral ($f_1=f_{\text{H,foam}}=0.9$) and collagen ($f_2=f_{\text{col,ultra}}=0.5$) contents typical of mature cortical bone, and three different values of the dispersion parameter δ of the r.v.s (assumed to be the same for all the r.v.s), namely $\delta=0.05$ (green lines), 0.1 (blue lines) and 0.2 (red lines). A total of $N=10^4$ computations were performed. It is apparent that, whatever the value of δ , the mean of the values of $Y_{\text{ultra},3}$ converges to the deterministic value (black dashed line). By contrast, the dispersion of the of values of $Y_{\text{ultra},3}$ does not converge to the corresponding input value of δ . Interestingly, the dispersion of $Y_{\text{ultra},3}$ is always smaller than that of the input r.v.s. Results obtained for the other elastic coefficients are similar but even more pronounced (data not shown).

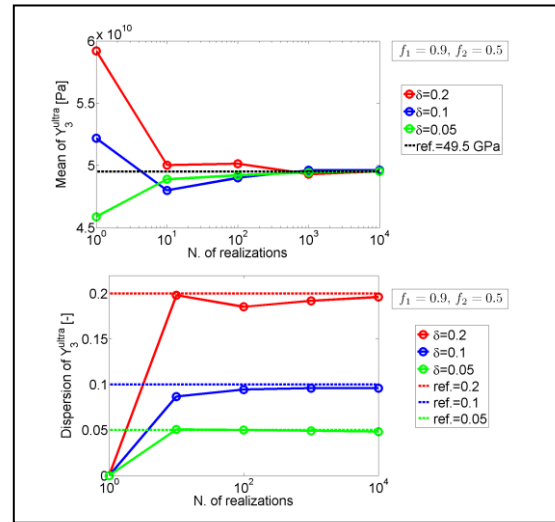


Figure 2 Running mean (top) and dispersion (bottom) of $Y_{\text{ultra},3}$. See text for details.

4. Conclusions

Lack of patient-specific data makes deterministic modeling of bone mechanical properties unreliable. The stochastic multiscale approach proposed in this paper allows estimating bone mechanical properties based on a few available data while preserving robustness of modeling. Statistical indicators (such as the dispersion or the confidence interval) can provide useful information on the reliability of the numerical results.

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