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The finite element method for micro-scale modeling of ultrasound propagation in cancellous bone

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ABSTRACT

Quantitative ultrasound for bone assessment is based on the correlations between ultrasonic parameters and the properties (mechanical and physical) of cancellous bone. To elucidate the correlations, understanding the physics of ultrasound in cancellous bone is demanded. Micro-scale modeling of ultrasound propagation in cancellous bone using the finite-difference time-domain (FDTD) method has been so far utilized as one of the approaches in this regard. However, the FDTD method accompanies two disadvantages: staircase sampling of cancellous bone by finite difference grids leads to generation of wave artifacts at the solid–fluid interface inside the bone; additionally, this method cannot explicitly satisfy the needed perfect-slip conditions at the interface. To overcome these disadvantages, the finite element method (FEM) is proposed in this study. Three-dimensional finite element models of six water-saturated cancellous bone samples with different bone volume were created. The values of speed of sound (SOS) and broadband ultrasound attenuation (BUA) were calculated through the finite element simulations of ultrasound propagation in each sample. Comparing the results with other experimental and simulation studies demonstrated the capabilities of the FEM for micro-scale modeling of ultrasound in water-saturated cancellous bone.

1. Introduction

Quantitative ultrasound (QUS) methods have been studied and clinically established for non-invasive assessments of bone status [1,2]. The capabilities of QUS techniques, in the context of osteoporosis, have been shown through prospective studies predicting the risk of fracture of the proximal femur, the vertebrae and hip and favorable results have been reported [3]. The clinical goal of QUS in the fields of bone assessment and osteoporosis diagnosis is to develop a tool for: (1) a reliable diagnosis of osteoporosis, (2) identification of subjects with high fracture risk and (3) sensitive monitoring of skeletal changes overtime [4]. To accomplish this goal, many in vitro and in vivo studies have been done over the past 40 years and a great variety of commercial QUS devices for bone assessment has been released over the past two decades [5,6]. However, the method has not yet achieved its ultimate applications especially as reliable diagnosing and monitoring techniques. The capabilities of the QUS methods depend on the interpretations of the QUS parameters i.e. speed of sound (SOS) and broadband ultrasound attenuation (BUA) with respect to bone status. Nevertheless, the interpretations of the parameters, supposed to unveil the correlation between the estimated parameters and bone status, still lack comprehensiveness [2,7]. The main obstacle to fully reliable interpretations of the measurements is reported to be the insufficient understanding of ultrasonic wave propagation in cancellous bone being a porous, heterogeneous and an isotropic medium [1,8]. Understanding the physics of wave propagation in cancellous bone is significant since osteoporosis mainly occurs at cancellous bone sites [9].

The physics of ultrasound propagation in cancellous bone has been studied utilizing in vitro approaches (like the immersion transmission experiments) for more than 40 years to find correlations between ultrasound parameters and physical and mechanical properties of cancellous bone samples [10]. In addition to the experimental methods, theoretical approaches with great potentialities in performing parametric studies have been proposed for exploring the wave propagation in the bone. The theoretical

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frameworks having been proposed for this purpose during the last two decades are Biot's theory [11–16] stratified or multi-layer models [17–19] scattering model [20], and micro-scale models [1,2,14,21–26].

Micro-scale models of cancellous bone are based on virtual geometries of trabecular networks spatially sampled and served as discrete domains of numerical simulations. The geometry of a trabecular network is either virtually reconstructed by employing micro computed tomography (μ-CT) images [1,2,14,21–26] or through developing geometrical models imitating a trabecular network [27,28]. The micro-scale modeling was proposed as an alternative to the other approaches since they achieved only some moderate success in explaining the physics of the wave propagation [1,21,29]. Accounting for the complex details of micro architectures of cancellous bone saturated with fluid, the micro-scale modeling has been reported to produce evidently more realistic results than that of the other methods [2,14,24]. The capabilities of this method regarding simulating experimentally observed wave propagation phenomena in cancellous bone-like the existence of two compressional waves, linear behaviour of the frequency-dependent attenuation and the correlations between the bone bulk density and the estimated ultrasound parameters – are the evidence for its advantages over the other methods [1,2,21].

Despite the advantages of numerical simulation of ultrasound propagation in cancellous bone using micro-scale modeling, discrepancies between the numerical and experimental results have been reported [1,2,22,25]. One of the sources of the discrepancies can be reasonably claimed to originate from the numerical method utilized in the micro-scale modeling. Briefly, the micro-scale modeling has employed the finite-difference time-domain method (FDTD) for its numerical approach to solve the linear wave equations governing the ultrasound propagation in the bone. In this approach, FDTD has used a Cartesian grid to spatially discretize the complex and heterogeneous micro-geometry of cancellous bone containing solid and fluid volumes.

A Cartesian grid leads to staircase sampling of the complex bone-fluid boundary (Fig. 1). Producing a jagged interface, staircase sampling generates unwanted wave artifacts in the solution [30]. The simplest remedy that can mitigate the errors originating from the staircase sampling is using a fine global grid. Evidently, this approach may not be practically and computationally efficient in the case of resolving the geometry of trabecular network. Other alternatives for resolving the sampling issue of boundaries which are not aligned with a Cartesian finite difference grid are local grid refinement [31], quasi-Cartesian grid [32], curvilinear grids [33], contour-path (locally deformed grid) algorithm [34], conformal FDTD techniques [35–40]. Each of these approaches has advantages and limitations for FDTD simulating elastic wave propagation; nonetheless, to the knowledge of the authors, their implementations in the case of wave propagation in trabecular structures have not been reported yet.

On the other hand, FDTD method should deal with the material discontinuity and their interfacial interaction at the solid–fluid interface [41]. The appropriate true physical interface condition for the simulations in which the saturating fluid is assumed as water (like in immersion transmission experiment) is perfect-slip.[3] The condition regarded as an acoustic–solid interaction should impose the inter-continuity of normal component of displacement (or velocity) at the interface, the equality of acoustic pressure in the fluid and normal traction in the solid at their shared boundary, and zero shear stresses (tangential component of the traction) at the interface in the solid medium [42]. The acoustic–solid interaction condition can be explicitly or implicitly imposed at the boundary grid points [41,43–45]. The explicit approach to the interfacial condition (also called homogeneous approach) has been generally developed. However its application is restricted to interfaces with simple geometry as horizontal, vertical or inclined line or plane boundaries [41,44]. This approach is impractical to 3-D curve material discontinuity interfaces; especially like the interface separating water/marrow and trabecular structures [41,44,46]. Even it becomes difficult or rather impractical in 2-D cases with curved boundaries since the scheme contains line integrals of the wave field [47] and also the geometry of the boundary must be known as a function of the Cartesian coordinates [41,47].

An alternative approach called the heterogeneous method, implicitly applies the physical acoustic–solid interaction condition at the interface. This method uses effective media parameters for the grid nodes located on the interface [30,42]. Effective media parameters are effective first Lame constant and effective density. These parameters are obtained by spatial averaging or combining the solid and fluid parameters in the vicinity of the interface. The true physical interfacial interaction is not necessarily satisfied by assigning the effective media parameters to the boundary nodes; however, its reliability is assumed [44]. The heterogeneous approach is associated with the first-order velocity-stress finite difference formulation of the wave propagation equation. This formulation is used with staggered grid and reported to be vulnerable to instability when the medium possesses high contrast material discontinuities [48]. The analyses for simulating the application of QUS in bone assessment [1,2,14,21,25–27,49] are mostly based on velocity-stress FDTD formulation on staggered grids; and although not reported, some kind of effective parameters at the fluid-bone interface must have been implemented. Therefore, it is reasonable to blame some part of the observed discrepancy (between simulation and experimental results) on the FDTD approach for the numerical solution of the wave equations in the complex medium.

One of the approachable remedy that can be claimed to be more efficient – than FDTD – in manipulating the complex geometry, material discontinuity and the acoustic–solid interaction in cancellous bone media is the finite element method (FEM). The FEM, reported to be generally superior to FDTD for elastic wave propagation analyses [50,51], can potentially account for better geometrical-sampling of any complex geometry [43]. Consequently, it should reduce the possible wave propagation artifacts arising from non-smooth sampling of fluid–bone interface. Regarding the material discontinuity and the interaction, the advantage of FEM over FDTD methods is that the acoustic–solid interaction condition can be explicitly satisfied at the interface [52].

It is worth mentioning that other researchers have already demonstrated that the micro-geometry of a trabecular network can be virtually reconstructed and prepared for static- or harmonic-load finite element analyses [53–56]. The models used either brick (8-node) elements or tetrahedral (4-node) elements to discretize the trabecular micro-geometry. In contrast to brick elements which led to stepwise (staircase) sampling of trabecular micro-geometry, tetrahedral elements generated a linear piecewise smooth approximation of the geometry. The latter even allowed generating a secondary interacting finite element volume-mesh filling the space between trabecular networks [53].

In the case of ultrasound propagation analysis, the FEM has been employed to simulate the wave propagation in a homogeneous micro-geometry of cancellous bone [57]. The simulations employed brick elements and did not consider any saturating fluid between the trabecular networks; hence unable to account for wave attenuation. Furthermore, other studies utilizing FEM to simulate the wave propagation in this field did not explicitly involve the micro-geometry of cancellous bone [7,58].

Although the FEM is theoretically developed enough for elastic wave propagation analysis and commercial software packages

[3] Perfect-slip conditions occur at a solid-fluid interface if there exists (or is assumed) no interfacial friction.