Finite-difference computation: a numerical tool for ultrasonic bone characterization

P. Laugier[a,*] E. Bossy[b], F. Jenson[a], M. Talmant[a], Frédéric Padilla[a]

[a]*Université Pierre et Marie Curie, Laboratoire d'Imagerie Paramétrique UMR CNRS 7623, 75006 Paris, France*
[b]*ESPCI, Laboratoire d'Optique UPR CN RS 5, 75005 Paris, France*

Abstract

Our objective here is to show the usefulness of computational methods in the field of ultrasonic bone strength characterization. Recently developed methods based on finite differences offer a fertile alternative to inextricable analytic formulations. Such numerical simulations of wave propagation have been applied to the problem of cortical axial transmission along the radius and transverse transmission through cortical bone (phalanx) or through cancellous bone (calcaneus). In each case, modelling has been found to be of great value in giving insight into the interaction mechanisms and properties of propagating waves (nature, pathway). Numerical simulation has already brought answers to the following issues: influence of complex 3-D geometry on ultrasound measurements, role played by structural anisotropy, sensitivity of axial transmission to porosity and cortical thickness. In the future, it will also provide insight into the role played by mechanical anisotropy, structural and mechanical heterogeneity, trabecular microstructure and physical loss mechanisms.

Keywords: Bone; Finite differences; Osteoporosis; Propagation; Ultrasound

1. Introduction

The rapid increase of incidence of fractures with age is related to several alterations in bone properties, such as reduction in bone mass and changes in its spatial distribution, increase in porosity, and modification of the bone matrix material itself. To encompass the multiple aspects of bone fragility, quantitative ultrasound (QUS) technologies have been proposed [1]. The nature of the information on bone properties conveyed by ultrasonic measurements has been a central question for many years [2].

An accurate interpretation of ultrasound measurements requires first a detailed understanding of ultrasound propagation with clear identification of the different waves that contribute to analyzed signals and their exact propagation path. Ultrasound propagation involves different types of waves in the medium (bulk compression or transverse waves, surface waves and guided modes) and several different interaction mechanisms (fluid–solid structure coupling, scattering, absorption, mode conversion). In addition, the nature of the problem differs depending on the skeletal site (cortical or cancellous bone) and the technique (transverse transmission or axial transmission). Therefore, ultrasound assessment of bone is complex and depends on a variety of skeletal parameters as well as on the experimental configuration. Because there is no unique comprehensive analytical framework to treat such a variety of problems, our objective here is to show the usefulness of computational methods in the field of ultrasonic bone strength characterization.

2. Materials and method

Simulations were performed using a finite-differences code, which computes a numerical solution to the three-dimensional (3-D) linear elastic wave propagation. Basically, the algorithm is based on spatial and temporal discretization of the following first-order equations:

$$\frac{\partial v_i}{\partial t} = \frac{1}{\rho(\mathbf{r})} \times \frac{\partial T_{ij}}{\partial r_j} \tag{1}$$

* Corresponding author. Tel.: + 33 1 44 41 49 60; Fax: +33 1 46 33 56 73; E-mail: Laugier@lip.bhdc.jussieu.fr

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$$\frac{\partial T_{ij}}{\partial t} = C_{ijkl}(\mathbf{r}) \times \frac{\partial v_k}{\partial r_l} \quad (2)$$

where r is the position vector, v the displacement velocity, T the stress tensor and C the stiffness tensor.

Equations (1) and (2) are written using Einstein's convention for implicit summation, with all subscripts varying from 1 to 3. This set of nine equations fully describes propagation in non-absorbing, heterogeneous, anisotropic and elastic media. The discretization of these equations according to the Virieux scheme [3,4] was chosen for its ability to accurately model propagation for both fluids and solids, and for a convenient implementation of perfectly matched layers (PML) [5] on the sides and edges of the simulation mesh, which is essential to efficiently avoid unphysical numerical reflections.

Three-dimensional (3-D) numerical simulations can be performed on actual bone geometry, as measured from computed tomography (CT) for instance, combined with local effective stiffness coefficients and density. Whereas low resolution X-ray CT data can be used to compute simulations at the level of a whole bone (organ level), high-resolution synchrotron radiation micro-CT (SR-μCT) data will be indicated to investigate the phenomena at the level of the microstructure, for example to document the impact on measurements of trabecular network microstructure or intracortical porosity.

For the purpose of our simulations, the bone matrix itself was considered to be a solid homogeneous material (isotropic or transversely isotropic) with effective stiffness and density according to values found in the literature [6,7]. In the future, however, properties at the tissue level could also be derived from high resolution imaging modalities such as scanning acoustic microscopy (SAM) for the stiffness coefficients [8] or synchrotron radiation micro-computed tomography (SR-μCT) for the density [9]. This will open the route to simulations that will include both material and structural heterogeneity.

3. Results

Cortical axial transmission – Axial transmission techniques have been developed to assess cortical bone properties [10]. Briefly, the axial transmission consists of recording with a set of receivers the propagation along the long axis of the cortical shell of an ultrasonic wave sent by a set of emitters aligned with the receivers on the same side of the investigated skeletal site. As an illustration, a typical 3-D snapshot obtained by entering into the software a real 3-D CT reconstruction from a human radius is shown in Fig. 1. What the numerical simulation brought here was an insightful view into the influence of intracortical porosity and cortical thickness on signal velocity. Cortical porosity leads to a decrease of the sound velocity at a rate of approximately $-25\ \mathrm{m\,s^{-1}}$ per % of porosity increase [11], which is consistent with experimental results [12]. In addition, the data show that the acoustical anisotropy of bone is partly explained by the anisotropy of the porous network. The variations of sound velocity as a function of cortical thickness predicted by finite differences simulation [11] are also in good agreement with *in vitro* and *in vivo* observations [13,14]. The sensitivity of signal velocity to cortical thickness (Fig. 1) has been clearly related to a change in the nature of the propagating wave [11] from a

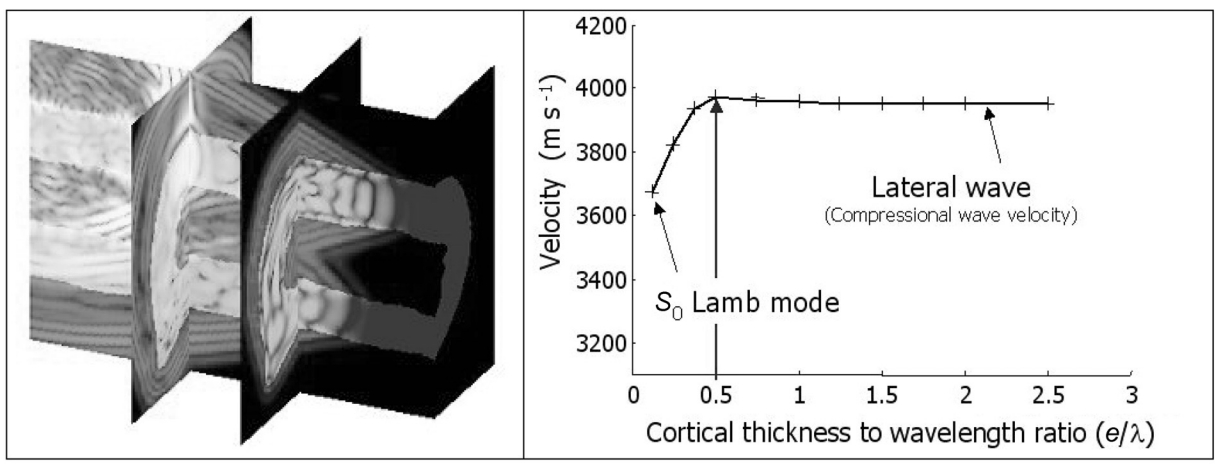

Fig. 1. 3-D snapshot (left) of ultrasonic waves propagating through a real cortical bone geometry obtained from 3-D X-ray computerized tomography. Impact of cortical thickness on signal velocity (right).

compression wave (the lateral wave) to a guided mode (equivalent to the S_0 Lamb mode in a plate model).

Cortical transverse transmission – Another direct application appears with cortical transverse transmission through the finger phalanges. The metaphysis of human phalanges consists in an irregular cortical shell surrounding the medullar canal filled with marrow. It is placed between two transducers (emitter and receiver) in a face-to face configuration. The metaphysis interacts with the incident wave, generating complex multiple pathways. Numerical simulations of the sound propagation through a model of cross section of a real human phalanx clearly demonstrates that the incident wave front is partly refracted as a wave propagating in the cortex along a curved pathway, while another pathway originates in the longitudinal wave transmitted at almost normal incidence through the medullar canal (Fig. 2). A part of the incident wave front also propagates through soft tissue alongside the cortex. Finally, mode conversion or multiple wave reflections occurring on interfaces give rise to multiple additional late arrivals at the receiver. Time intervals between signals following different pathways and relative signal amplitudes are influenced by material and structural (porosity) properties and by bone morphology (cortical cross-sectional area, area of the medullar canal, cortical thickness). Numerical simulations were very helpful to document the influence of these bone characteristics on quantitative measurements. While the velocity of the fastest signal mostly depends on the cortical cross-sectional area, the amplitude depends mostly on the area of the medullar canal [15].

Transverse transmission through cancellous bone – Clinical devices that measure in transverse transmission the speed of sound (SOS) or broadband ultrasound attenuation (BUA) of cancellous bone at the heel (calcaneus) are now widely used and evidence lends support to their use for the assessment of fracture risk [16,17]. While cortical bone can be viewed in a first approximation as a dense continuous solid at the scale of the wavelength (millimeter scale), trabecular bone cannot be regarded as homogeneous but rather as a highly porous material, including a solid framework of connected rod-like or plate-like trabecular elements, with soft tissue in the pore spaces.

The interplay between fluid-like marrow and the solid trabecular network causes loss mechanisms such as scattering, viscous friction and mode conversion, providing a plausible interpretation for the observed high attenuation level. Contribution of viscous losses and scattering to total attenuation have been debated many times, while mode conversion or even different mechanisms such as energy dissipation in the interconnected trabecular network as a whole received no attention. Three-dimensional finite differences computations running on 3-D data sets obtained from SR-μCT (Fig. 3) can be used to clarify the contribution of scattering and tissue absorption to frequency-dependent attenuation, a widely used parameter for assessing bone. Such simulations are currently being performed on 3-D numerical models of bone, obtained from human calcaneus specimens (N = 38) previously assessed experimentally by transverse transmission [18]. Comparison between numerical predictions and experimental

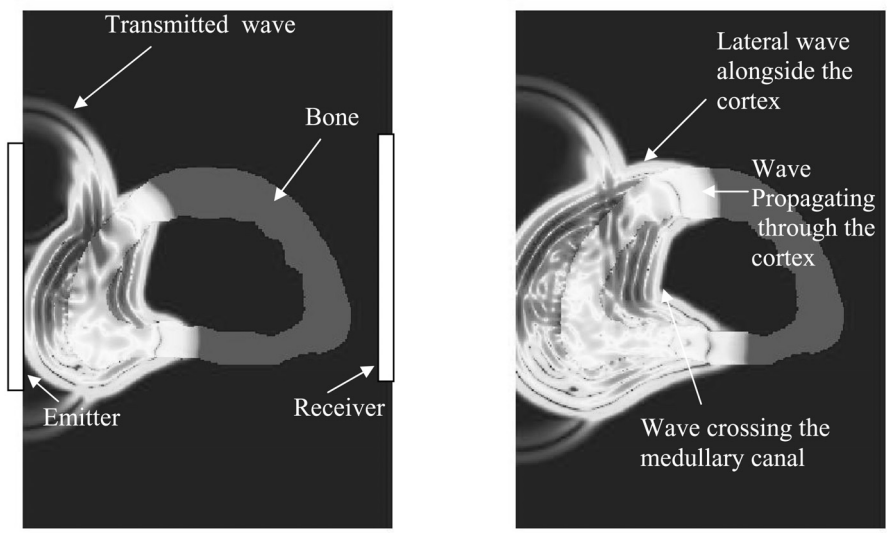

Fig. 2. Snapshots illustrating the transmission of a plane wave through the phalanx (20, 30 μs) and the multiple pathways.

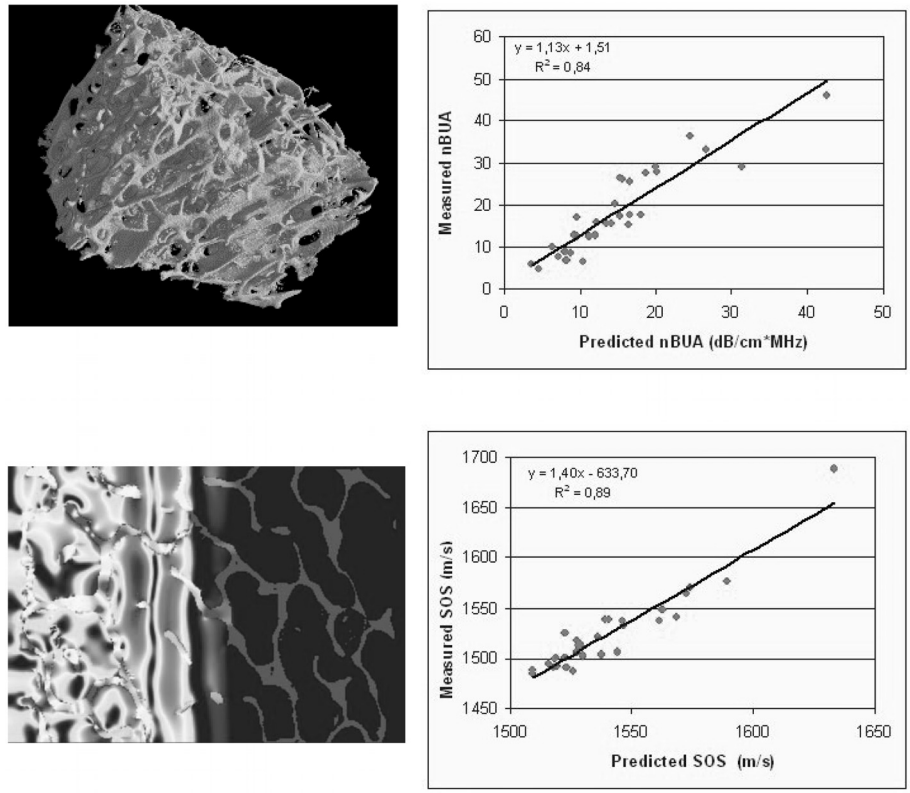

Fig. 3. Snapshots (bottom left) illustrating the propagation through a 3-D numerical model of cancellous bone (top left). Scatter plot of measured BUA against predicted BUA (top right). Scatter plot of measured SOS against predicted SOS (top right).

(Fig. 3) showed an excellent agreement. Because the numerical model does not include any tissue absorption at all, the data strongly suggest scattering and conversion modes as serious candidates to explain total losses.

4. Discussion

It is virtually impossible to model by analytic means the extremely complex field resulting from the interaction of an incident wave with bone taking into account the full complexity of boundary conditions, geometry, heterogeneity in bone properties and the diversity of experimental conditions. Recently developed simulation methods based on finite differences offer a fertile alternative to inextricable analytic formulations. Such numerical simulations of wave propagation have been applied to the problem of axial transmission along the radius [11] and transverse transmission through the phalanx [13] or through cancellous bone (calcaneus). In each case, modelling has been found to be of great value in giving insight into the interaction mechanisms and properties (nature, pathway) of propagating waves. Numerical simulation has already brought answers to the following issues: influence of complex 3-D geometry on QUS measurements, role played by structural anisotropy, sensitivity of axial transmission to porosity and cortical thickness. In the future, it will also provide insight into the role played by mechanical anisotropy, structural and mechanical heterogeneity, trabecular microstructure, physical loss mechanisms, etc.

Numerical simulations can be conceived as a tool for virtual experimentation to quickly and efficiently test unedited experimental configurations, to design novel clinical instruments (e.g. ultrasound tomography) and, ultimately it is hoped, to refine measurement protocols to enhance fracture risk prediction.

It can be used to elucidate the relationship between QUS variables and bone material and structural properties and to test inverse calculation procedures. In particular, it can assist experimental studies, which are inherently limited by the ever-increasing difficulty in collecting human sample sizes large enough to be representative of a population with a given pathological status (e.g. osteoporotic, non-osteoporotic, etc.). One way of overcoming this difficulty would be in the future

to perform virtual experiments using three-dimensional data sets reconstructed from high-resolution imaging acquisition (e.g. SR-μCT). This would allow, from a limited number of specimens, the testing of several scenarios of virtual micro-architecture alteration (*in silico* osteoporosis) and the independent study of the effects on QUS variables of various bone characteristics that pertain to bone strength.

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