MULTISCALE MODELING OF BONE FRACTURE AND STRENGTH

Allocation: Illinois/50 Knh
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EXECUTIVE SUMMARY:

We are using Blue Waters to run a multiscale computational model of bone fracture and strength. Fracture is a multiscale phenomenon with cracks initiating at the atomic level. Thus, we are modeling bone as a biological material with a hierarchical structure spanning from the atomic level (crystal structure of minerals and atomic structure of collagen), to nanoscale (mineralized collagen fibril), sub-micron scale (single lamella), microscale (lamellar bone), mesoscale (cortical and trabecular bone types), and macroscale (whole bone) (fig. 1). We are conducting atomic- and nanoscale-level simulations using molecular dynamics software NAMD with CHARMM and LAMMPS and higher scales by employing finite-element software Abaqus. The inputs are taken from experiments. This will be the first experimentally based multiscale modeling of bone fracture and strength. Blue Waters is necessary because such multiscale model requires very high computational resources due to the hierarchy of bone structure and complex fracture phenomena in bone.

INTRODUCTION

We are using Blue Waters to test a novel multiscale computational approach to predict fracture and strength of normal versus osteoporotic bone. Osteoporosis is a bone disease characterized by low bone density and deterioration of bone structure leading to bone fragility and increased risk of fractures [1]. In the United States osteoporosis is a major public health threat for an estimated 44 million people. It is a silent disease with no symptoms prior to fractures and no cure, but treatments can slow its progress. Thus, early and accurate diagnosis is crucial. Currently, bone quality is assessed clinically by measuring the bone mineral density, although other factors such as bone's complex hierarchical structure (fig. 1) also contribute to bone's properties. A new approach is sorely needed for more accurate diagnosis of osteoporosis. A computational mechanics model can provide a new tool for the clinical assessment of bone.

About Bone Structure

Bone is a multifunctional biological tissue that has an ideal combination of properties when healthy: high stiffness, strength, and fracture toughness, and light weight. These superior properties are due in part to the complex hierarchical structure of bone from macroscopic (whole-bone) to atomistic levels [2] (fig. 1). At the mesoscale, one step smaller than the macroscale, bone tissue is composed of the dense cortical bone and the spongy trabecular bone. Mature human cortical bone consists of osteons embedded in an interstitial bone and surrounded by a circumferential bone, whereas the trabecular bone is made of a porous network of trabeculae. At the microscale both cortical and trabecular bones have lamellar (layered) structures formed through stacking of lamellae in different orientations. At the sub-microscale a single lamella is made of preferentially oriented mineralized collagen fibrils perforated by ellipsoidal cavities called lacunae. At the nanoscale the mineralized collagen fibril is a composite structural unit consisting of the collagen, nano-sized hydroxyapatite crystals, water, and a small amount of non-collagenous proteins. The sub-nanoscale represents the atomistic scale of bone's constituents: tropocollagen molecules and crystals.

Similarly, bone strength and fracture is a very complex phenomenon with different failure mechanisms exhibited at different structural scales (fig. 2). They include crack deflection and twist, uncracked ligament bridging, collagen fibril bridging, and constrained micro-cracking.

Furthermore, there are two types of toughening mechanisms in bone (fig. 3): 1) *intrinsic* mechanisms that act ahead of the crack tip and increase the microstructural resistance to crack initiation and growth, and 2) *extrinsic* mechanisms that act primarily behind the crack tip to inhibit crack growth by effectively reducing the crack-driving force actually experienced at the crack tip.

METHODS & RESULTS

The objective of this study is to test a complex 3D multiscale model of bone strength and fracture. Modeling starts at the atomistic level and moves up the scales to the macroscale. Atomic- and nanoscale-level simulations are done using the molecular dynamics software NAMD with CHARMM and LAMMPS, and larger scales were added using the finite-element software Abaqus. We have preliminary results from molecular dyanmics and obtained properties of collagen molecules. We are now finalizing our nanoscale model that can feed in the data for the larger-scale model.

At the sub-microscale we are modeling bone as a collection of mineralized collagen fibrils. We are generalizing an elastic-case model to use in a nonlinear case with deformations up to fracture. We have already modeled lamellar bone at the microscale and are currently simulating trabecular bone up to failure with the goal of obtaining anisotropic constitutive models for the macroscale. At the macroscale we are modeling a whole human femur.

This research is in collaboration with Dragomir Daescu from Mayo Clinic. We received the image of the whole femur bone from Mayo Clinic. We will be using this geometric model for our multiscale simulations. Our preliminary models of bone elasticity and strength are given in [3–5].

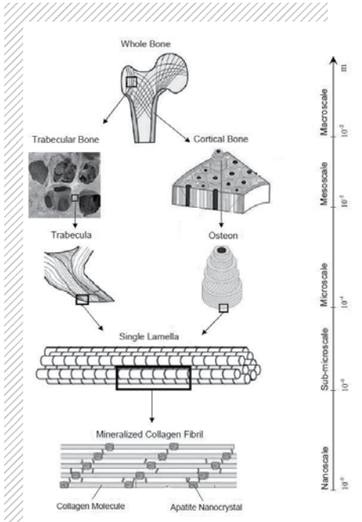

FIGURE 1: Hierarchical structure of bone.

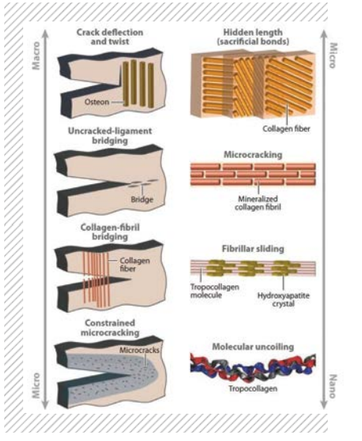

FIGURE 2: Different fracture and failure mechanisms in bone.

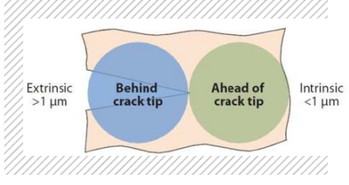

FIGURE 3: Two types of toughening mechanisms in bone.

WHY BLUE WATERS?

All these factors make bone fracture and strength a very complex and highly computationally intensive problem to study. The modeling requires a multiscale approach accounting for all these different structural features and failure modes. Such a model is intractable using current high-end computers. Thus, Blue Waters is crucial for such computations. No comprehensive multiscale model yet exists in the literature due to these computational challenges and limitations.