Project Title: MULTISCALE MODELING OF BONE FRACTURE AND STRENGTH

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- ## Executive summary

In this project, nonlinear finite element models of trabecular bone were used with the aim of building a predictive tool to model plasticity and strength of this biological material. The complex, random, and irregular features of bone were effectively captured using micro-computed tomography images to build three-dimensional finite element models with up to 10 million degrees of freedom. The direct multi-frontal solver in Abaqus/Standard with hybrid Message Passing Interface (MPI)/Threaded parallelization was used to analyze the models. The complexity of the structure, material and geometric nonlinearities, along with complex contact conditions make the numerical analysis very challenging even on the latest high performance computing platforms. Our results show close match with experimentally measured stiffness and strength and our model was also able to capture experimentally observed plasticity of the trabecular bone demonstrating the potential of the model to predict mechanical behavior. This computational model serves as a crucial step in multiscale modelling of whole bone.

- ## Description of research activities and results

Osteoporosis which is a growing clinical problem in aging societies is a bone disease characterized by low bone density and deterioration of bone's structure leading to bone fragility and increased risk of fractures [1]. It is a silent disease with no symptoms prior to fractures and no cure, but treatments can slow its progress. Thus, its early and accurate diagnosis is crucial. Currently, bone quality is assessed clinically by measuring the bone mineral density while other factors such as bone's complex hierarchical structure also contribute to bone's properties. Thus, a new approach is needed for the more accurate diagnosis of osteoporosis. Computational mechanics model can provide an effective new tool for the clinical assessment of bone health.

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Bone is a multifunctional biological tissue, which among its other functions, serves as a structural support for soft tissues in the body. As a structural material it has an ideal combination of properties when healthy: high stiffness, strength, and fracture toughness, and light weight. Bone is made of a stiff cortical bone forming an outer core and a spongy trabecular bone filling an inside space and ends of long bones. Such geometry is optimal as it minimizes weight, reduces bearing stresses at joints, and allows the body to withstand high functional loads. These superior properties are due in part to the hierarchical structure of bone ranging from molecular to macroscopic levels [2]. These structural scales are described in Fig. 1.

The macroscale represents the whole bone level. At the mesoscale the bone tissue is composed of the dense cortical bone and the spongy trabecular bone. The mature human cortical bone consists of osteons embedded in an interstitial bone and surrounded by a circumferential bone. The trabecular bone is a highly porous, heterogeneous, and anisotropic mineralized tissue made of a network of trabeculae. At the microscale both cortical and trabecular bones have lamellar 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 type I, nano-sized hydroxyapatite crystals, water, and a small amount of non-collagenous proteins. The sub-nanoscale represents the atomic scale of bone's constituents: tropocollagen molecules and crystals [2, 3].

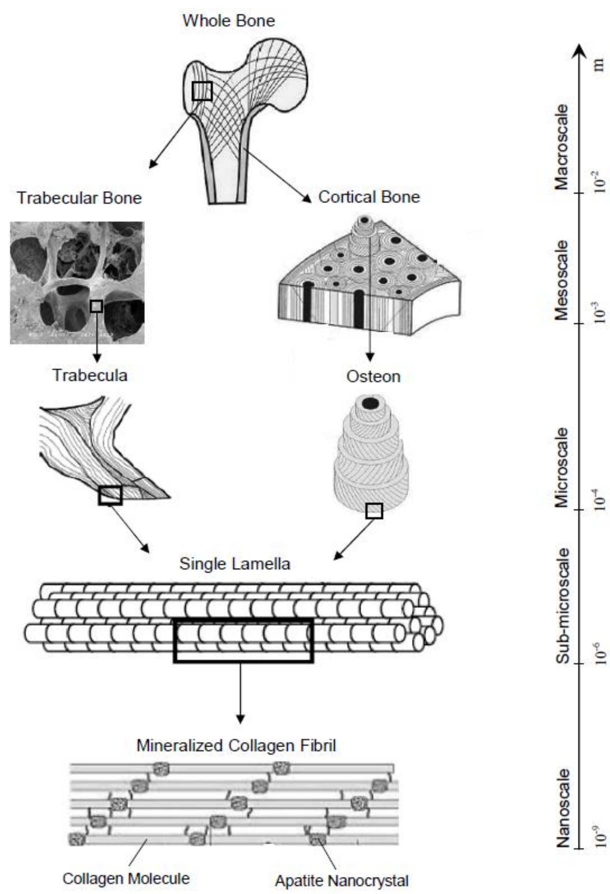


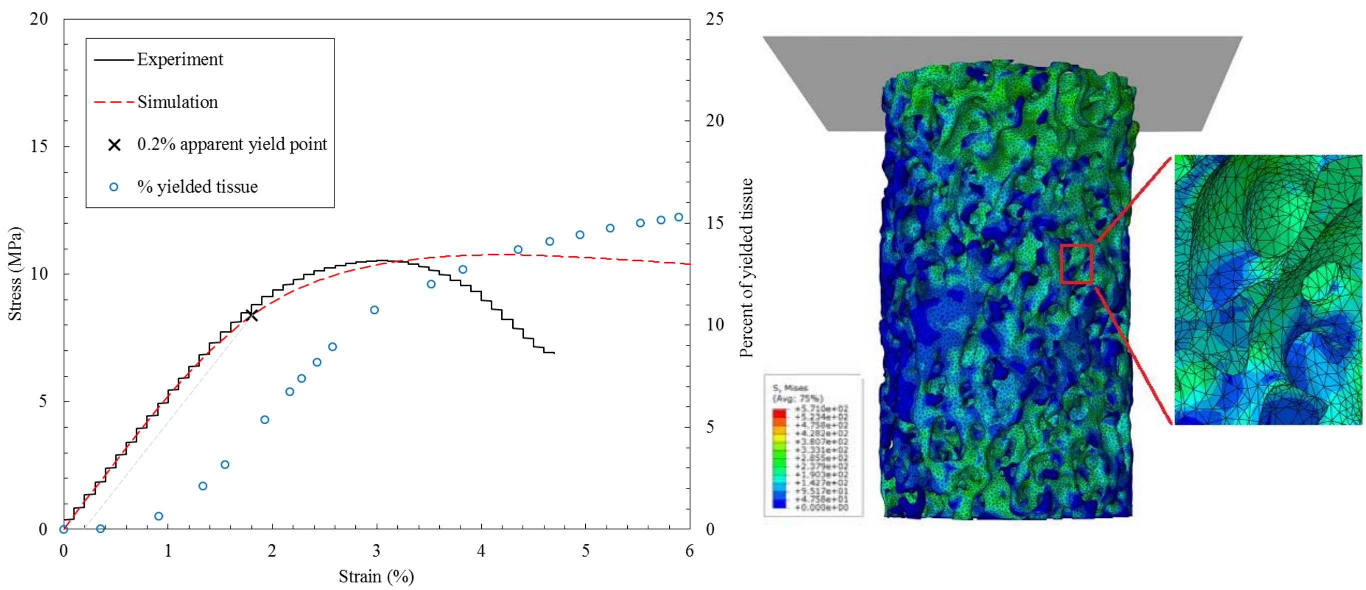
Fig 1. Hierarchical structure of bone

Dense cortical bone and porous trabecular bone work together to provide excellent load-bearing properties of bone. Osteoporosis-related fractures, mostly occur in trabeculae-rich areas of bone. Trabecular bone is also the primary site for insertion of orthopedic implant systems. Thus, mechanical properties of trabecular bones are of high clinical and research interest for prediction of age- and disease-related bone fractures, optimizing treatments to reduce fracture risks, as well as designing improved implant systems [4-6]. In this project, trabecular bone was simulated using non-linear finite element (FE) models to gain better understanding of its mechanical behavior. Such models have the potential to build a structure-based predictive tool to assess strength and damage locations of patient-specific samples. It can also serve as a guide to engineers for design of novel synthetic bio-mimetic and bio-inspired materials for a wide range of engineering applications.

In this project, nonlinear micro-computed tomography (micro-CT) FE model of trabecular bone was built as a cost-effective alternative to experiments and conventional methods that are costly, time-consuming and prone to several artifacts. In this model, the complex, random, and irregular features of bone microstructure were captured with the microstructure data obtained from micro-CT imaging. The model was then meshed and analyzed under loading that involved numerical simulations on very large random microstructures of trabecular bone. Each model included up to 10 million degrees of freedom.

There are two mechanisms underlying the nonlinear behavior of trabecular bone: nonlinear elastic behavior due to finite deformations of the highly porous structure, and the material nonlinearity of the tissue due to damage and plastic deformations [5, 7, 8]. Huge number of degrees of freedom, material and geometric nonlinearities, along with complex contact conditions make the numerical analysis very challenging even on the latest high performance computing platforms. Within each quasi-static time step, a system of nonlinear equations was linearized and solved with a Newton-Raphson (NR) iteration scheme [9, 10] in Abaqus which required several linear solver solutions or global equilibrium iterations. The direct multi-frontal solver in Abaqus/Standard with hybrid Message Passing Interface (MPI)/Threaded parallelization was used. Abaqus license is generously provided on Blue Waters as a courtesy of NCSA's Private Sector Program. Analysis of the models was done utilizing up to 256 CPU cores and large memory capabilities of the Blue Waters. Dr. Koric [11] has recently shown that the similar multifrontal solver had enough scalability and robustness to perform computations on large ill-conditioned FEA problems on many thousands of CPU cores, thus potentially opening the door for future higher fidelity and complexity simulation studies in biomechanics.

An example of our trabecular bone FE model along with a comparison between simulations and experimental at apparent level (whole sample level) are presented in Fig. 2. Our results show a close match with experimentally measured stiffness and strength. Plasticity of the trabecular bone model is also well captured in our simulations showing the potential of the model to predict mechanical behavior. The effectiveness of micro-CT FE models as predictive tools for mechanical properties of trabecular bone is directly dependent on proper calibration and validation. As such, as part of this project, influence of using different constitutive laws and parameters at the tissue level on apparent response was investigated through a systematic study to serve as a guide for modeling trabecular bone. These results are published in the following conference and journal articles.



(a) **(b)**

Fig 2. Apparent stress-strain curves from experiment and simulation along with percent of yielded tissue, b) Example of von Mises stress distribution in samples under uniaxial compression [12]

- List of publications associated with this work

S. Koric, F.A. Sabet, O. Jin, I. Jasiuk, (2016) "*Direct numerical simulation of bone plasticity and strength*" International Symposium on Plasticity, January 2016, Keauhou, Hawaii.

F. A. Sabet, O. Jin, S. Koric, I. Jasiuk, (2016) "Nonlinear micro-CT FE modeling of trabecular bone – Sensitivity of apparent response to tissue constitutive law", submitted to Journal of the Mechanical Behavior of Biomedical Materials.

F.A. Sabet, D. W. Abueidda, E. Hamed, O. Jin, S. Koric, I. Jasiuk, (2016) "Hierarchical modelling of plasticity and strength of trabecular bone," to be presented at XXIV ICTAM, 21-26 August, 2016, Montreal, Canada.

S. Koric, F.A. Sabet, I. Jasiuk, (2018) "Influence of tissue level plasticity on apparent response of trabecular bone" International Symposium on Plasticity, January 2018.

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[12] F. A. Sabet, O. Jin, S. Koric, I. Jasiuk, “Nonlinear micro-CT FE modeling of trabecular bone – Sensitivity of apparent response to tissue constitutive law”, submitted to *Journal of the Mechanical Behavior of Biomedical Materials*.