ADVANCED DIGITAL TECHNOLOGY FOR MATERIALS AND MANUFACTURING

Allocation: Exploratory/50 Knh
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EXECUTIVE SUMMARY

This exploratory Blue Waters proposal provided the computing resources to four graduate students, funded by the NCSA Materials & Manufacturing (M&M) group, to explore how their research can be furthered through the use of advanced digital technology to address large-scale problem solving. Two of the four research activities conducted via the allocation are reported below.

The first project, titled "Simulation of Reference Point Indentation on Cortical Bone," was conducted by Ashraf Idkaidek. He used two different instruments that utilize the Reference Point Indentation technique—BioDent and Osteoprobe. The second project—"Mechanics of Materials with a Focus on Accelerated Design and Structure-Processing-Property Relations of Materials via High-Scale Computations"—was conducted by Fereshteh A. Sabet. In this work, he investigated and compared the performance of implicit and explicit solvers for trabecular (inner layer) bone using Abaqus.

Project 1—Simulation of Reference Point Indentation on Cortical Bone

RESEARCH CHALLENGE

Osteoporosis is a bone disease responsible for two million broken bones and $19 billion per year in related costs in the United States, alone. By 2025, osteoporosis is expected to be responsible for three million fractures and $25.3 billion in related costs per year, according to the U.S. National Osteoporosis Foundation. Assessing the relationship between bone fracture resistance and bone material properties is important for the diagnosis and treatment of bone diseases. Using traditional material testing approaches such as compression, tension, or three- and four-point bending to measure bone mechanical properties is *ex vivo* and destructive.

METHODS & CODES

Cortical bone forms the outer hard shell of the whole bone. Therefore, understanding cortical bone fracture behavior is essential to evaluate whole-bone fracture resistance. The Reference Point Indentation (RPI) technique was invented to allow *in vivo* evaluation of bone properties. There are two instruments that use the RPI technique: BioDent and Osteoprobe. BioDent applies multiple indents at the same location on cortical bone, whereas Osteoprobe applies only one loading cycle at multiple neighboring locations on cortical bone. The relationship between RPI and bone properties has not been developed and is still an open topic.

In our research, we are focused on numerically relating both BioDent and Osteoprobe RPI instrument outputs to actual bone material mechanical properties. The cortical bone RPI simulation problem (using the commercial Abaqus software) is highly nonlinear where geometric nonlinearity, material nonlinearity, and contacts are needed to be accounted for to preserve the accuracy of the simulation results.

RESULTS & IMPACT

We have related each of the 10 outputs of the BioDent RPI instrument to bone material properties by using the finite element method [1]. We have also evaluated the simulation of bone fracture using the extended finite element method on a single-osteon cortical bone sample [2,3]. Further, we are currently developing a study to relate Osteoprobe RPI output to bone material properties and fracture resistance.

WHY BLUE WATERS

Completing this study is fully dependent on the numerical finite element method. The problem is highly nonlinear, and multiple iterations are needed to relate Osteoprobe device output to different bone mechanical properties. Each of the Osteoprobe RPI simulation iterations demands high computational power and time. Therefore, completing such a study using multicore Blue Waters clusters is essential.

PUBLICATIONS & DATA SETS

Idkaidek, A., and I. Jasiuk, Toward high-speed 3D nonlinear soft tissue deformation simulations using Abaqus software. *J Robot Surg*, 9:4 (2015), pp. 299–310.

Idkaidek, A., and I. Jasiuk, Cortical bone fracture analysis using XFEM—case study. *Int J Numer Method Biomed Eng*, 33:4 (2017), DOI:10.1002/cnm.2809.

Idkaidek, A., S. Koric, and I. Jasiuk, Fracture analysis of multi-osteon cortical bone using XFEM. *Computational Mechanics*, 62:2 (2018), pp. 171–184.

Project 2—Mechanics of Materials with a Focus on Accelerated Design and Structure-Processing-Property Relations of Materials via High-Scale Computations

RESEARCH CHALLENGE

Bone has a hierarchical architecture spanning from atomistic to macroscopic scales. At the scale of one to a few millimeters, the bone tissue is composed of cortical (outer) and trabecular (inner) bone. Osteoporosis is a bone disease characterized by low bone density, which often leads to an increased risk of fractures that mainly occur in trabecular bone. Trabecular bone is also the primary site for insertion of orthopedic implant systems. Thus, the mechanical properties of trabecular bone are of great clinical and research interest for prediction of age- and disease-related fractures, as well as the design of improved implant systems [1,2].

METHODS & CODES

Modeling of trabecular bone entails a highly nonlinear mechanical behavior along with contacts. This leads to increased ill-conditioning of global stiffness matrices and difficulties converging, especially in the post-yield regime [3]. As a result, it is of considerable interest to assess the effectiveness and efficiency of an explicit solution method. In this project, we used the implicit and explicit solvers of Abaqus to analyze nonlinear micro-Computed Tomography (micro-CT) finite element (FE) models of trabecular bone and compared the performance of the two solvers.

RESULTS & IMPACT

Our results show that, by using a similar setup for the model (e.g., element type, loading type, etc.) when using implicit and explicit solvers, there is a perfect match between micro-CT FE model results using implicit and explicit solvers. Fig. 1 shows an example of stress–strain curves obtained from nonlinear micro-CT FE modeling of trabecular bone using implicit and explicit solvers along with experimental results. As can be observed, with the explicit solver we are able to reach a higher applied strain without convergence difficulties. There is also a good match between local stresses obtained using implicit and explicit solvers, as shown in Fig. 2. In addition, we observed that implicit and explicit solvers scale similarly, while the explicit solver performs five times faster.

WHY BLUE WATERS

We were able to successfully scale our simulations on eight to 12 nodes on Blue Waters with the explicit solver, which significantly reduced computational time. Each of our models has many millions degrees of freedom and nonlinearities, making them impossible to solve without the use of the Blue Waters supercomputer.

PUBLICATIONS & DATA SETS

Sabet, F.A., O. Jin, S. Koric, and I. Jasiuk, Nonlinear micro-CT based FE modeling of trabecular bone—Sensitivity of apparent response to tissue constitutive law and bone volume fraction. *International journal for numerical methods in biomedical engineering*, 34:4 (2017), p. e2941.

Sabet, F. A., S. Koric, and I. Jasiuk, A comparison between implicit and explicit finite element simulations of trabecular bone. In preparation (2018).

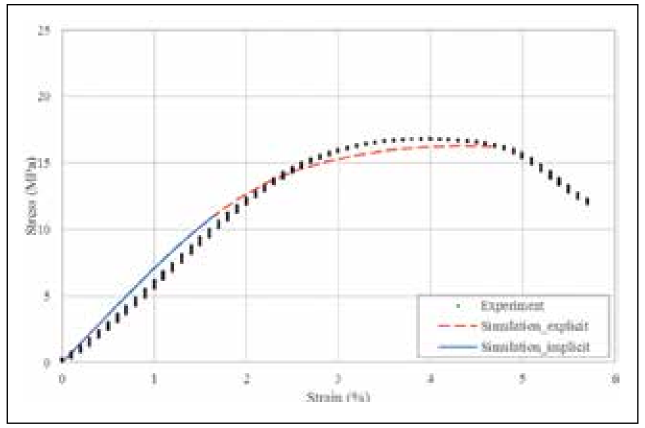

Figure 1: Comparison of apparent response resulting from implicit and explicit solvers (*Project 2*).

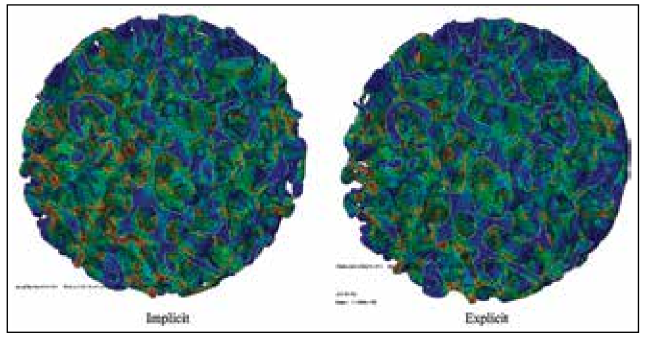

Figure 2: Comparison of contact pressure obtained using implicit and explicit solvers (*Project 2*).