TN

BW

MP

ADVANCED DIGITAL TECHNOLOGY FOR MATERIALS AND MANUFACTURING

Allocation: Exploratory/50 Knh
PI: Ahmed Taha[1]
Co-PIs: Seid Koric[1], Sudhakar Parmidighantam[1,2], Narayan Aluru[3], Gabrielle Allen[1,3]
Collaborators: Ashraf Idkaidek[3], Shantanu Shahane[3], Fereshteh A. Sabet[3], Ethan Shapera[3]

[1]National Center for Supercomputing Applications
[2]Indiana University
[3]University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY

This exploratory Blue Waters (BW) proposal provided computing resources to four graduate students funded by the National Center for Supercomputing Applications Materials & Manufacturing group, allowing the students to explore how their research can be furthered through the use of high-performance computing to address large-scale problem-solving. Two of the research activities that used the BW allocation, both involving analysis of bone, are reported here.

The first project, titled "Simulation of Reference Point Indentation on Cortical Bone," was conducted by Ashraf Idkaidek. He used two different instruments—BioDent and Osteoprobe—that utilize the Reference Point Indentation (RPI) technique. The second project, "Mechanics of materials with focus on accelerated design and structure-processing-property relations of materials via high scale computations" was conducted by Fereshteh A. Sabet. This project examined and compared the performance of implicit and explicit solvers for modeling trabecular bone using Abaqus.

Project 1 - Simulation of Reference Point Indentation on Cortical Bone

RESEARCH CHALLENGE

Bone has a hierarchical architecture ranging from atomistic to macroscopic scales. At the scale of one to a few millimeters, the bone tissue is composed of cortical and trabecular bone. Osteoporosis is a bone disease characterized by low bone density, which leads to an increased risk of fractures that occur mainly 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 for designing improved implant systems.

METHODS & CODES

Modeling of trabecular bone entails highly nonlinear mechanical behavior along with contacts. As a result, it is of considerable interest to assess the effectiveness and efficiency of explicit solution methods. In this project, we used the implicit and explicit solvers of Abaqus to analyze 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 there is a good match between micro-CT FE model results using implicit and explicit solvers (see Fig. 1). We also observed that implicit and explicit solvers scale similarly, but 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 saved computational time. Each of our models has many millions of degrees of freedom and nonlinearities, making such models impossible to solve without the use of a supercomputer.

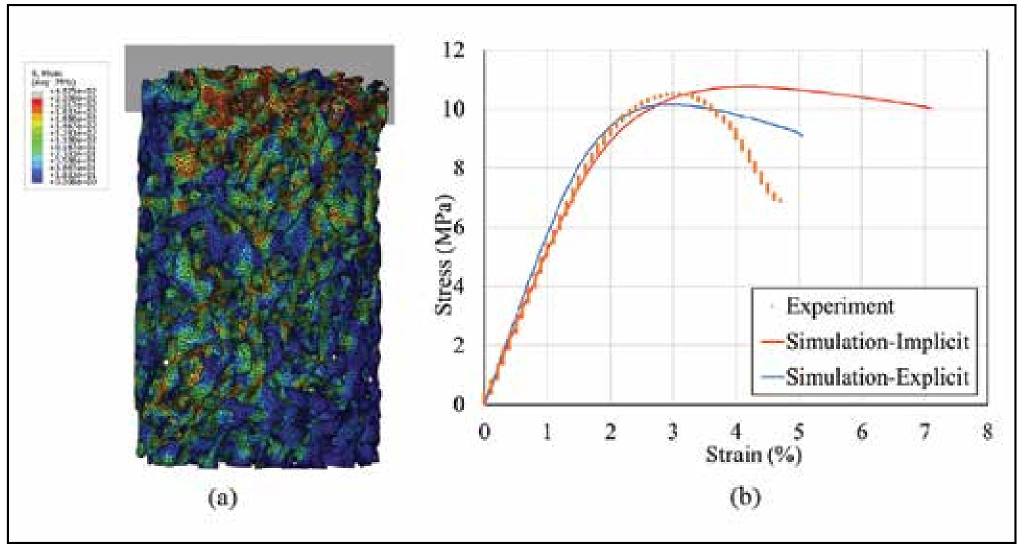

Figure 1: Project 1—(a) Example of von Mises stress distribution in samples under uniaxial compression, (b) implicit and explicit solver results versus experimental stress–strain curves.

Project 2 - Mechanics of materials with focus on accelerated design and structure–processing–property relations of materials via high-scale computations

RESEARCH CHALLENGE

Osteoporosis is responsible for two million broken bones at a cost of $19 billion, annually in the United States. According to the National Osteoporosis Foundation, by 2025 this disease is expected to lead to three million fractures at a cost of $25.3 billion per year. Assessing bone material properties in relation to its fracture resistance is important for the diagnosis and treatment of bone diseases. Using traditional materials testing approaches to measure the mechanical properties of bone, such as compression, tension, and three-point and four-point bending, are *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 fracture resistance of the complete bone. The Reference Point Indentation (RPI) technique was invented to allow *in vivo* evaluation of bone properties. Two different instruments 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 is highly nonlinear, where geometric nonlinearity, material nonlinearity, and contacts must be accounted for in order to preserve the accuracy of simulation results. We use Abaqus software to simulate cortical bone RPI.

RESULTS & IMPACT

Relating each of the 10 outputs of the BioDent RPI instrument to the bone material properties has been established using the finite element method [1]. Also, simulating bone fracture using the extended finite element method on a single-osteon cortical bone sample has been evaluated and published [2]. A study to relate Osteoprobe RPI output to bone material properties and its fracture resistance is currently being developed.

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 be able to relate Osteoprobe device output to different bone mechanical properties. Each Osteoprobe RPI simulation iteration demands high computational power and time. Therefore, completing such study using the multi-core BW system is essential.

PUBLICATIONS AND DATA SETS

Idkaidek, A., V. Agarwal, and I. Jasiuk, Finite element simulation of Reference Point Indentation on bone. *Journal of the Mechanical Behavior of Biomedical Materials*, 65 (2017), pp. 574–583.

Idkaidek, A., and I. Jasiuk, Cortical bone fracture analysis using XFEM—case study. *International Journal for Numerical Methods in Biomedical Engineering*, 33: e2809 (2016), DOI: 0.1002/cnm.2809.