MULTIPLE SCALE MODELING FOR PREDICTIVE MATERIAL DEFORMATION ANALYSIS

Motivation. Material deformation and stress-strain is an active area of mathematical modeling relevant to industrial and research-oriented materials science. It is important to take variations in material properties into account in these models. Multi-scale models that incorporate inhomogeneity were studied and modeling frameworks that address this need were created and tested. Incorporating variations in material properties at the micro scale resulted in significantly different predictions of material deformation under similar loading. Variations in material properties were accounted for through averaging over stresses in representative volume elements (RVEs). This project was a collaborative effort by students, **Rachel Aronow**, **Aaron da Silva**, **Rose Dennis**, **Abdel Kader Geraldo**, **Dean Katsaros**, **Melissa Sych**, and **Richard Touret**, under the guidance of Professor **Qian-Yong Chen**.

Background. In material science, the deformation of materials under tension is an important problem with widespread application. Using the stress/strain equations as the basis for the model, material properties are encoded, and the model is solved to predict behaviors of real-life materials. The material properties are encoded via the material's Poisson ratio, and its young's modulus. Young's modulus is defined mathematically as the ratio of the tensile stress to the strain. Poisson's ratio is the ratio of the transverse strain to the axial strain. Simply, Young's modulus is the measure of material stiffness, and Poisson's ratio the tendency of the material to expand perpendicular to the direction of compression.

It is important to note that a material may not have the same Poisson ratio or Young's modulus in different parts of the material. We say that this is an inhomogeneous material. Commonly, deformation models assume homogeneity in the material being modeled. The homogenous version of these stress/strain equations is much easier to solve. However, this assumption leaves important characteristics of the material out of the model. This motivates taking a multi-scale approach to modeling the material.

The multi-scale approach incorporates the inhomogeneity of a material via combining a macro and micro-scale set of equations. Both equations assume homogeneity, but the micro-scale equations have different property coefficients corresponding to their location. Representative Volume Elements (RVEs) is the name given to the micro-scale units. This project investigated the differences in modeling results when a multi-scale approach is taken.

Tissue Mechanical Testing. To investigate the effects of multiscale modeling, we chose to focus on the problem of a ligament under uniaxial tension testing, as performed by Chokandre et al. in 2015. In particular, ligaments are an inhomogeneous material. The uniaxial tension test performed in this study is described as follows: a 1 mm x 4.46 mm dumbbell-shaped sample of tissue from an MCL (0.53 mm thick) is clamped at both ends and stretched slowly, such that the internal forces in the tissue remain balanced (quasi-static equilibrium). At each time step, the force applied to the tissue and the tissue's resulting displacement is recorded.

To model this experiment, we used the plane stress/strain equations. These equations are given by:

$$\nabla\cdot(\sigma) = F \qquad \sigma = D\epsilon \qquad \epsilon = \nabla\cdot U$$

where $U=[u,v]$ is displacement, $\epsilon=[\epsilon_x,\epsilon_y,\tau_{xy}]$ is strain, $\sigma=[\sigma_x,\sigma_y,\tau_{xy}]$ is stress, $F=[F_x,F_y]$ is the internal body force (set to zero), and D is a coefficient matrix describing the elasticity of the material. D is dependent on E and v, and is easy to calculate for a homogenous material. These equations are derived from the following assumptions:

1. The problem is two-dimensional
2. The material is homogenous and its elasticity can be described fully by two parameters: Young's Modulus, E and Poisson's Ratio, v
3. The material is in equilibrium (stresses are balanced throughout the material)

Using MATLAB and the open source toolbox FEATOOL (https://www.featool.com/), we defined a 1 mm x 5 mm rectangular region as our ligament. With the data from Chokandre et al. (2015) in hand, we calculated an average Young's Modulus (slope of the stress vs. strain curve) of the MCL (E=36 MPa) and used this to describe the elasticity of our simulated material. For a Poisson's ratio, we adopted a typical value for an MCL (v=0.02) from Sweigart & Athanasiou (2005). Assuming quasi-static equilibrium, we set the initial displacement of the material to be 0 and applied a forcing of 1.3 N in the positive y-direction to the top edge (Figure 1). To simplify the model, we assumed symmetry and set the bottom edge to be held fixed. These conditions were enforced via boundary conditions. Solving the plane stress equations via the finite element method results in the displacements displayed in Figure 2. We observe that the top edge of the region is displaced 0.27 mm, compared to a displacement of ≈0.45 mm observed in the data set.

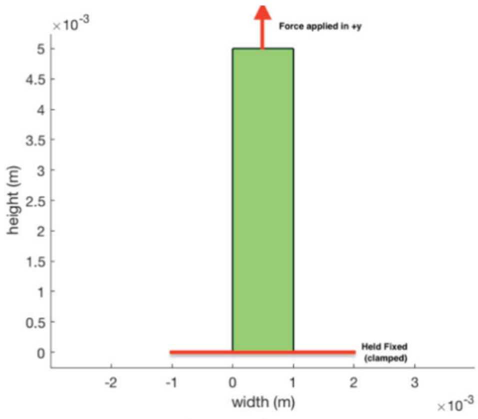

Figure 1.

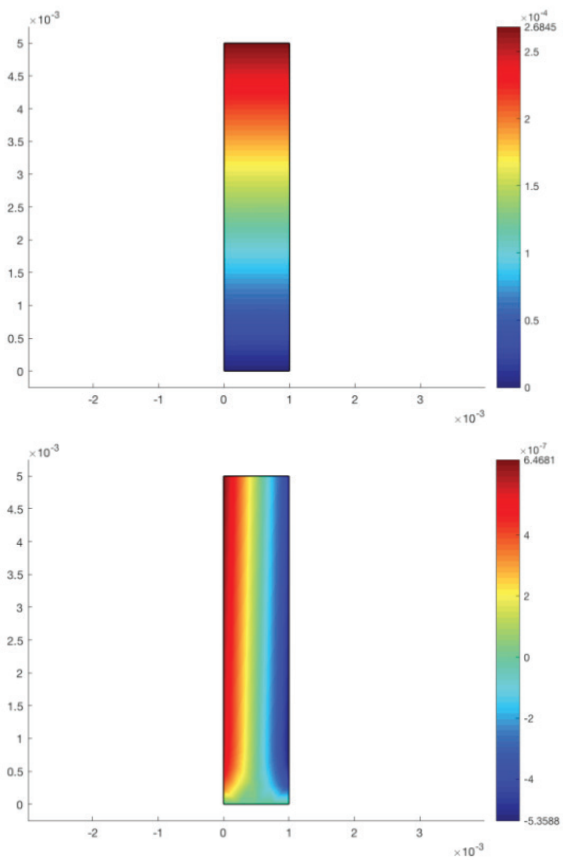
Figure 2. (y displacement left, x displacement right)

Multiscale Modeling Approach. In order to solve the force balance equations, we had to make the assumption that the entire ligament is homogenous. However, some of the most exciting potential applications of biomechanics apply to problems involving in-homogenous materials. For example, we consider a ligament with an "injury" point, in order to incorporate a multi-scale approach to the problem.

One Macro-Region. For a benchmark, we first solved the problem for the simple homogenous case. As in Section 2, we used the average values of E and v across the whole body. Again, the initial displacement and internal forcing (body force) were set to 0, and a 1 N upwards forcing was applied to the top edge while the bottom edge was held fixed. Then the plane stress/strain equations were solved using the finite element method. These steps were repeated until the material stabilized its shape. The solution was then interpolated for the entirety of the region using MATALB's scatteredInterpolate function. The resulting deformation of the material is shown in Figure 3. Qualitatively, the material behaves as expected under tensile stress.

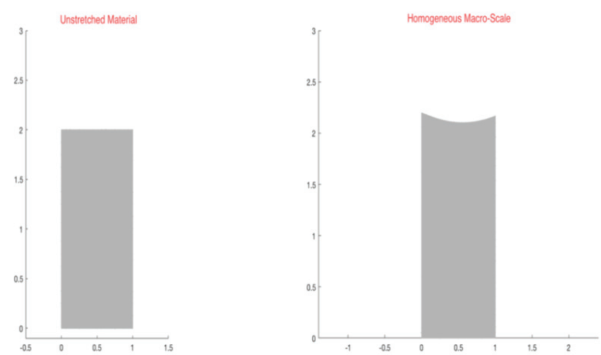

Figure 3.

For our second model, we introduced four RVEs, located at the Gauss points of the rectangular macro-region. The RVE in the top right corner was given a lower Young's Modulus and greater Poisson's ratio than the rest of the material, to indicate a point of poor stability (see insert in Figure 4). We then applied a multi-scale approach based off Barocas (2007), and summarized as follows: We first solved one iteration of the macro-problem as described in Section 3.1. We then solved the plane stress equations in each homogenous RVE for the stress resulting from the external loading. For this step, we used boundary conditions interpolated from the closest macro-region boundary to the RVE. Next, we calculated Q, as introduced in Barocas (2007). The Q factor is defined by the volume average of $Q_{RVE(k)}$ where k refers to the indexing of the RVEs and $Q_{RVE(k)} = \frac{1}{Vol_{micro}} \int (stress_{RVE(k)} - AvgStress_{macro}) d\mu(x)$. We then resolved the plane strain equations in the macro-region, but with the internal forcing set to Q instead of 0. This captures the effect of inhomogeneity on the internal forcing of the material, and thus how it responds to an external forcing. We continued to switch between calculating Q in the micro-scale problem and balancing forces in the macro-scale problem until the solution stabilized. The result of this simulation is shown in Figure 4.

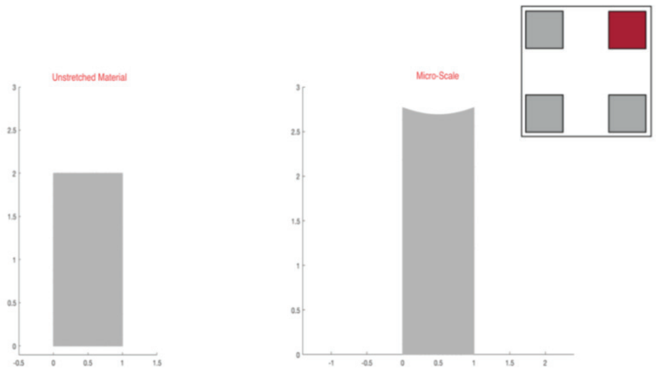

Figure 4.

Multiple Macro-Units with a Microscale. To include finer detail in the model, we introduced a grid of four macro-regions, each containing four RVEs at their Gauss points. We therefore have sixteen locations to introduce inhomogeneity. The top and bottom edges of the ligament, where the tissue is anchored to the bone, were set to be slightly less elastic than the overall material, and the injury point was set to be more elastic, representing an instability point in the fiber alignment. Starting with the top left macro-unit, we complete one iteration of the method described in Section 3.2. We then repeated the process for the top right macro-unit, with the additional boundary condition of the stress along the right edge of the top-left macro-unit being equivalent to the stress felt by the left edge of the top-right macro-unit. Continuing clockwise, we then solved the problem for each of the bottom units in a similar manner. This process was then repeated until the solution stabilized.

Results & Discussion. A comparison of the three simulations is shown in Figure 5. Incorporating the microscale in the second simulation affects the magnitude of the deformation, but not its shape. This is an issue inherent to our method. The microscale is represented by the Q factor, which behaves like a weighted average of the relative stress felt in each RVE. This term was then used as an internal forcing term, and so a positive Q value forces the body in the same direction as the external force, meaning the same magnitude external force can displace the material further. Therefore, this model does not capture any information about the location of the fine details, just the existence of a more flexible region within the tissue.

The model with multiple macro-units however, does demonstrate a change in both the magnitude and shape of the deformation. The lopsided tissue shows signs of the location of the injury point. Although the effects of the micro-units are still averaged together to find Q, there is now a Q factor for each macro-region, therefore holding on to structural details within each macro-unit. Thus, the introduction of multiple macro-units is better at encoding fine details, without losing all the details to averaging.

One of the challenges to multi-scale modeling is the lack of a rigorous benchmarking method. Our results show that incorporating a micro-scale changes the shape of the deformation, but we do not possess the data sets to determine which model is "best."

Furthermore, the way the microscale stresses are incorporated into the macro scale should be examined in future work. The Q factor is a counterintuitive way to do this, as it is an averaging process. The degree to which the microscale is detailed can become computationally impractical very quickly, so some sort of approximation is necessary. However, it is not clear whether there is a better approximation than the Q factor.

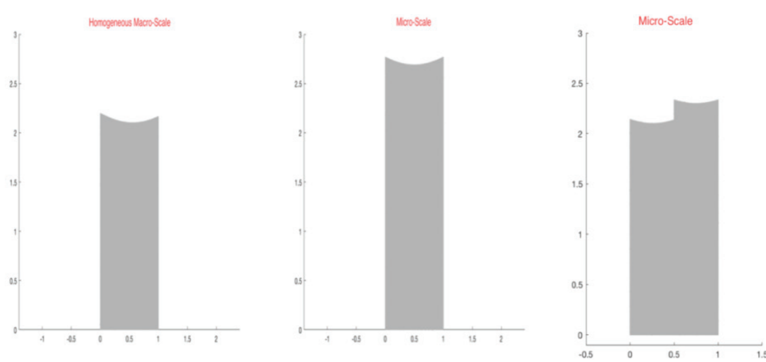

Figure 5.

Conclusion & Future Work. Incorporation of the microscale causes different deformation behavior. This reflects the importance of taking into account the heterogeneous nature of many materials. For more comprehensive studies to be productive, the benchmarking of these models needs to be more rigorous. Benchmarking should not necessarily be reliant on imaging, as comparison of real images to experimental images can be ill-defined. The model could be made more robust in future studies by using fiber equations instead of stress-strain modeling. Here, microscale stresses would be calculated at cross-linking sites in the micro-scale, and these stresses would be factored into the plane stress at macro-scale, a computationally expensive approach.

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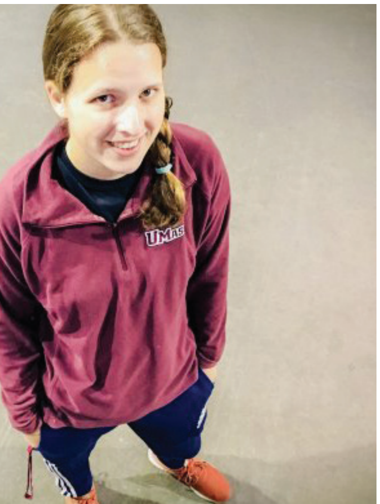

RISING RESEARCHER AWARD

Commonwealth Honors College student **Shelby Cox** '18 is a Mathematics & Statistics and Linguistics double major who has a track record of winning awards that reflect her superb academic performance and leadership abilities in the field of mathematics and statistics. Along with establishing and serving as President of the UMass chapter of the Association for Women in Mathematics, Cox has received two Outstanding Academic Achievement Awards from the Department of Mathematics and Statistics as well as the 2017 William F. Field Alumni Scholar Award, which recognizes and honors third-year students for their academic achievements. Shelby won a prestigious National Science Foundation graduate research fellowship to pursue a PhD in pure mathematics this fall at the University of Michigan.

Cox's research accomplishments began when she participated in a summer 2016 National Science Foundation Research Experience for Undergraduates (NSF/REU) at the University of Maryland. The project concerned calculating the Euler characteristic of geometric objects, known as Hilbert schemes, which are mathematical structures in algebraic geometry that occur under symmetry. The Euler characteristic is a rough measure of the topology, or shape, of an object. The heart of Cox's achievement was to reduce these calculations to previous known calculations that are more mathematically manageable. Cox and her collaborator gave a talk and also presented a poster on their work in January 2017 at the Joint Mathematics Meetings – the largest gathering of mathematicians in the United States and the largest annual meeting of mathematicians in the world.

According to Associate Professor Eric Sommers, her advisor and teacher, "Shelby's superb performance in research and departmental coursework, as well as her role in establishing and leading the UMass chapter of the Association for Women in Mathematics, makes her deserving of the Rising Researcher award."

Cox acknowledged just how much what it means to be a scientist has changed—but that the principles of science have remained the same:

> *As we move on to new adventures as educators, actuaries, data scientists, software engineers and researchers, we probably won't have to remember the pigeonhole principle or the first 10 digits of π, but we will continue to solve problems.*

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