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Finite Element Optimization of a Mechanical Device for Connecting Dissimilar Materials by Dong Hwan Yoon

A thesis presented to the School of Engineering of Washington University in St. Louis in partial fulfillment of the requirements for the degree of Master of Science

May 2018

Saint Louis, Missouri

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# Acknowledgments

Special thanks goes to Guy M. Genin, Stavros Thomopoulus, Victor Birman and Steve Linderman who have reviewed this thesis and helped support the related research.

Dong Hwan Yoon

Washington University in St. Louis

May 2018

#### **ABSTRACT OF THE THESIS**

Finite Element Optimization of a Mechanical Device

For

Connecting Dissimilar Materials

by

Dong Hwan Yoon

Master of Science in Mechanical Engineering Washington University in St. Louis, 2018 Research Advisor: Professor Guy Genin

The tendon to bone attachment is a major challenge from the surgical, mechanical, and tissue engineering perspectives. From the surgical perspective, repair is plagued with high failure rates. From the mechanical perspective, the attachment of two highly dissimilar materials, tendon and bone, poses a perennial challenge. From the tissue engineering perspective, surgical reattachment presents a major opportunity. In this context, this thesis explored how soft-to-hard tissue attachments occurs in animal predation. A two-dimensional simulation of a tooth was implemented in a commercial finite element program. The tooth varied in shape so as to vary from a canine shape to a python shape. Stress and displacement fields shifted as a function of shape, with python-like teeth showing special features that enhance gripping of the soft tissue.

# Chapter 1

## Introduction

The context in which this study was undertaken is the attachment of tendon to bone, which is a major challenge from the surgical, mechanical engineering, and tissue engineering perspectives [1-3]. For surgery, up to 94% of rotator cuff reattachments fail [4]. From the mechanical engineering perspective, the mechanisms of resilience at the insertion site are an area of ongoing research [5-11], and must overcome the free edge singularity problem [12-29]. From the tissue engineering perspective, the natural tendon to bone attachment does not grow back [4], and it is important to find ways to stabilize tissue without this attachment [20-23] and to guide regrowth of the transitional tissue [24-28]. Stabilization of tissue during healing is a topic that I am focusing on and have contributed to a conference paper on [29]. The question of resilience of tissues motivated my ongoing study of how carnivores capture and tear through flesh.

Carnivores have a broad variety of teeth, many of which are believed to be optimized for specific purposes [48]. For example, within the human mouth, molars are believed to be best optimized for grinding, and canines and incisors are believed to serve the function of biting and tearing. The dentition of a *Tyrannosaurus rex* is optimized for cutting, consistent with its supposed mode predation involving removal of chunks of flesh from its prey (Figure 1b). Some of the teeth are curved slightly, which I hypothesize to be for the purpose of helping hold onto chunks of flesh as the animal fed upon its prey. The dentition of a python, however, differs still further. Here, the teeth are curved still further back (Figure 1a.) This might be consistent with the predatory habits of the python, which swallows live animals whole. The jaws of the python become unhinged, and the teeth must serve a purpose that differs from those of the

*Tyrannosaurus rex.* Whereas the *Tyrannosaurus rex* removes chunks of flesh for the purpose of consumption, and possibly used its jaws as weapons to kill its prey by laceration or suffocation, the python's teeth must accomplish a diametrically different purpose. If the python teeth cut a chunk from the animal it hunts, the animal stands a chance of escaping. A reasonable hypothesis is therefore that the teeth of a python are designed to grip soft tissue without tearing.

Fascinating support for this hypothesis comes from the study of *Acomys*, also known as the African spiny mouse. This mouse has skin that is brittle and that tears off in chunks when it is stressed beyond a critical threshold [50]. The mouse is also fascinating from the perspective of regeneration, as it grows back this flesh without scarring. Even hair grows back in the injured regions of tissue. This feature is hypothesized to be an escape mechanism that might give the African spiny mouse an advantage in its efforts to avoid predation: by overcoming the gripping design of the python's teeth to turn them into teeth that tear. Clearly, this suggests that there is an interplay between tooth design and soft tissue material properties that can be tailored to change the specific function of a tooth.

The challenge of gripping instead of tearing underlies the problem of surgical reattachment of tendon to bone. Here, a key problem is that the sutures in a repair act like teeth that can tear through a reattached tendon early in the healing interval following a surgery, and thereby cause the surgery to fail through re-tearing of the tendon-to-bone enthesis. However, we know from recent work in the literature, including much work from my colleagues, that certain, sometimes subtle, changes to the material properties of a tissue can lead to dramatic changes in its toughness and its ability to resist tearing [51-60]. Such material changes are the subject of a tremendous body of work, and also of new technologies for surgical repair [55].

In this thesis, I address the opposite question, and ask whether teeth, or anchoring technology, might be optimized to make attachment of soft tissue more like a python and less like a *Tyrannosaurus rex*. The first step in this study was a review of basic solid mechanics solutions for curved beams [30], and a study in an introduction to finite element analysis [31] was done. The upshot of these was the realization that several features of the design of a tooth serve to mitigate high stresses in the tooth itself. However, it was clear from our preliminary analyses that structural failures such as buckling dominate over material failure in the design of teeth.

We therefore evaluated how teeth both stress and constrain soft tissues. The goal was to determine what shapes lead to high stresses at tooth tip, and what shapes lead to constriction of the soft tissue against a rigid gumline. The shape of the model was inspired from how a python tooth would capture its prey and lock on to it, and a range of teeth that span the shark-to-*Tyrannosaurus rex*-to-python spectrum was studied parametrically.



Figure 1a. Photo of Python Snake Skull that shows the curved shape of the teeth [47]. We hypothesize that a tooth-shaped hook can grip in the early stages of repair and insure a tight contact between the tendon and bone.

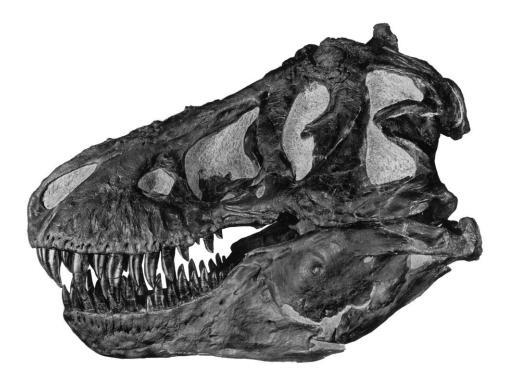


Figure 1b. Photo of a *Tyrannosarus rex* skull that shows the less curved shape of the teeth [48]. We hypothesize that a pyramid-shaped hook can tear flesh.

# Chapter 2

# Methods

Numerical simulations were performed to assess how teeth might be optimized to switch from cutting teeth that induce high principal stresses on an isotropic continuum to trapping teeth that induce compression of an isotropic continuum against a rigid simulated gumline. The first step in this study was a review of basic solid mechanics solutions for curved beams [30]. Thereafter, I evaluated how teeth both stress and constrain soft tissues. As mentioned above, the goal was to determine what shapes lead to high stresses at tooth tip, and what shapes lead to constriction of the soft tissue against a rigid gumline. The shape of the model was inspired from how a python tooth would capture its prey and lock on to it, and a range of teeth that span the shark-to-*Tyrannosaurus rex*-to-python spectrum was studied parametrically.

The numerical portion of the study was conducted using the finite element method, and using commercial software (Abaqus/CAE) for the analysis. The steps involved in a finite element analysis are coming up with an idealized geometry, assigning idealized material properties, choosing boundary conditions, making a mesh, implementing the boundary conditions, solving the equations (equilibrium, strain displacement, and constitutive equations) by a matrix-based energy minimization method, and then validating results by mesh refinement [31].

#### 2.1 Idealized geometry

Teeth were modeled parametrically to shift from a nearly pyramidal canine to a hooked pythonlike tooth. Analyses were performed under plane strain conditions. Each tooth was treated as a pair of splines that intersected at a curved top. The teeth were each of a base w and a height of 2*w*. The curvature of the tooth was determined by moving the tip (sharp end) to the right in the Abaqus/CAE sketch interface, thereby increasing the distance w' (Figure 2). The tooth has a dimension of 2 x 4 x 1 (length, height, width) in arbitrary units (in this study mm). The top region of the tooth from the left end to the tip is referred to w' and the base of the tooth is referred to w. The parameter that determines the degree of curvature can be expressed as w'/w where in this study ranges from 0.5 to 2.25 (Figure 2).

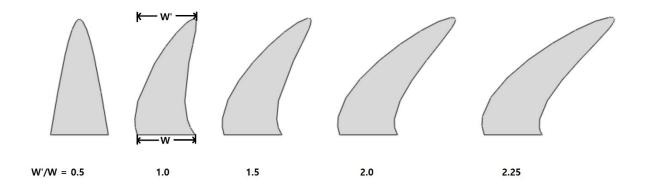


Figure 2. General view of tooth model with annotations of w and w'.

Clearly, setting the parameter as w'/w equal to 0.5 yielded a shape that is representative of the cross-section of a conical tooth. As the parameter w'/w increased, the tooth adopted a shape that was increasingly swept to the right, a direction meant to represent the direction from the mouth to the throat of an animal. A key outcome of the study was to determine the shape w'/w at which the response of the tissue penetrated by the tooth shifted from cutting to gripping, and another was to identify the limits at which the tooth began to "hook into" and potentially injure tissue through elevated principal stresses.

A tissue was placed over the tooth (Figure 3). The right and left boundaries of the tissues, placed a distance 4w away from the middle of the tooth. The height of the tissue was 4w away from the base of the tooth. A gumline was placed at the bottom of the tooth and was assigned the same

material properties as the tooth, described below. The tooth/gumline and the tissue were not allowed to interpenetrate.

#### 2.2 Material properties

The problems studied here were idealized teeth on an elastic foundation contacting with a softer material, which would ideally resemble a tendon. As a first approximation, the teeth and softer tissue were modeled as linear hyperelastic and as isotropic. The hyperelasticity was irrelevant for the tooth due to its high relative stiffness and strength. Also, the tooth was modeled as a solid rather than multilayered structure due to the stresses that were very small compared to its failure strength: the tooth was effectively rigid compared to the soft tissue. The Young's modulus and Poisson's ratio were set to 14 GPa and 0.3 for the tooth, respectively. These values correspond to human cortical bone which I have used as a reference material that would allow me to gain insight [32-36]. The values that were used can be changed easily which can be later analyzed when I have a firm idea on what the actual material will be used to create a device that would assist in the human rotator cuff repair.

The tendon properties were a Young's modulus of 0.14 GPa and Poisson's ratio of 0.3. These are reasonable values for tendon that is under tension [6-8], [14]. The isotropy of the tendon is a poor approximation in general, but is slightly better in cases when healing tissue is involved. [6-8]

#### 2.3 Boundary conditions

The boundary conditions were as follow. The base of the gumline and the tooth was restrained from moving. The right and left boundaries of the tissue were displaced a prescribed amount in the horizontal direction, and kept shear-free. The top boundary of the tissue was traction free. The lower boundary of the tissue and the portions contacting the tooth were shear free, meaning that there was frictionless contact between the tooth and tissue. The normal boundary condition (that is, in the direction normal to the tooth or gumline surface at a particular point) could shift from one of constrained displacement that prevented interpenetration to one of zero traction, depending on the solution. The solution procedure was therefore nonlinear not only because of the large strain kinematic framework employed, but also because of the need to iterate on this contact boundary condition.

The master-slave algorithm built into Abaqus was used for this purpose. This algorithm penalized interpenetration with a large, nonlinear interfacial stiffness in compression.

#### 2.4 Mesh

The models were two dimensional, and plane strain, linear interpolation quadrilateral and triangular elements were used.

Abaqus was used to refine the mesh until the strain energy and peak principal stress in a model did not change more than a few percent with additional refinement. The corresponding plots of the maximum principal stress, strain tensor energy and the strain energy density were studied.

The mesh size can be controlled through the graphical user interface in Abaqus/CAE. However for the purpose of this study the finer upper is the part which simulates the soft tendon, is the part of more interest, therefore used a finer mesh (Figure 3). The bottom part which resembles the tooth has a larger mesh. The graphic interface in Abaqus/CAE allows the user to change the mesh size and element type (quadratic or linear). For the purpose of this study, quadratic elements were used.

#### 2.5 Mesh refinement

The analysis was repeated for increasingly small mesh sizes until the peak principal stress ceased to change. A typical study required approximately 4 minutes of time on a modern laptop.

Note that the sharp tooth led to exceptionally high stress concentrations. The mesh convergence study therefore had to proceed with extra care. Additional confidence in these simulations was achieved by observing an asymptote in behavior of the model and associated stress and displacement fields as the parameter w'/w was varied.

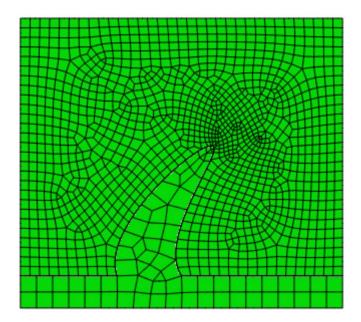


Figure 3. Example mesh of tooth and tendon model in contact

#### 2.6 Limit: Buckling

As the curvature increases, the length of the tooth also increases therefore the buckling effect had to be considered. As compressive load is applied to the tooth in the horizontal direction when seen from the top, the tooth may deflect which may cause unwanted problems to the tendon. To examine the effects of buckling, a top view of the tooth model was use and a horizontal load was applied to check the magnitude of deflection with respect to the curvature length w'/w.



Figure 4. Example mesh size of 0.1 of buckling model w'/w=9.5

# Chapter 3

### Results

Results showed that stresses in the tendon were highly localized to the tip of the tooth, with stress concentrations well above 10 at the contact point (Figure 11). This is consistent with the sharp nature of the rounded tip of a tooth, and is expected for an appendage that must penetrate tissue. In subsequent analyses, the objective was to determine the degree to which changes to the tooth affected the degree of this stress concentration. The deformed shape of the tendon and tooth model implies that the model created acts as expected. (Figure 12).

Before pursuing that further, the stress field within the tooth itself was explored. The maximum tensile principal stress follows what would be expected in a cantilever beam with the boundary conditions used. For the curved tooth, the tensile stresses were in general higher on the loaded face, and the principal stress was zero on the back face, consistent with what is expected for flexure of a beam [30]. In the simulations where the bottom boundary was "encastre" [31], meaning that the displacement was fixed to zero, a stress concentration known as a Williams free-edge singularity appeared at that corner [44]. The stress concentrations or stress singularities can be suppressed by choosing different boundary conditions, such as a foundation that is elastic in shear or a cohesive zone model, which is used in fracture studies [31,46]. This is where the rectangular base for the tooth model comes in to eliminate any singularities (Figure 6). Although the understanding of these mechanisms falls under multi-scale modeling that is beyond the scope of what is needed for this study, phenomenological models can be used to account for how microstructure relates to continuum behavior [45-46]. The second is an hourglass effect [31]. Here, the oscillatory nature of the free edge singularity shows up as a series of errors in the estimation of displacements, which makes neighboring quadrilateral elements look like

hourglasses [31]. The hourglass effect can be suppressed by choosing elements with "hourglass control" or by choosing triangular elements [31].

The normal strain in the vertical direction also shows what would be expected from Euler-Bernoulli beam theory (Figure 7). The strains are generally tensile on the loaded face and compressive on the free face. A strain concentration is evident at the curve of the curved tooth. Both teeth also show the free edge singularity at the point that is fixed.

We next explored the response of the tissue. The first value of interest was the maximum principal stress (S.Max.Prin. in the terminology of Abaqus). This was plotted normalized by the applied stress, which was estimated by summing the total nodal forces on the two vertical faces and dividing this by twice the cross-sectional area. These forces were found by evaluating the NFORC1 parameter returned by Abaqus.

At lower levels of curvature, the maximum principal stress reached an asymptote. Note that for values of the curvature parameter w'/w less than 0.5, the problem was not stable: the flesh would be fly off of the tooth without a top jaw crunching the flesh back downwards. Because this upper surface is not of interest in the biomaterial attachment problem studied, no values of w'/w less than 0.5 could be studied.

Beyond a critical value of the parameter w'/w, the already high peak principal stress concentration began to rise further. This was true for both levels of deflection studied, a displacement of .5% and 1% of w. For both of these cases, the critical value of the parameter w'/w was just over 1.5.

The next value of interest was how well the tooth forces the tissue onto the substratum. In the case of a tendon-to-bone healing scenario, an increased normal stress is advantageous for healing. The value studied was the average stress in the Y direction along the gumline (Avg.S22 in Abaqus), again divided by the average applied stress. This value was nearly zero for low values of the parameter w'/w, but then increased linearly with w'/w beyond a threshold of about w'/w=1.25.

Finally, the fraction of the tissue that was in contact with the gumline was studied. The contact area fraction increases as the curvature increases where it seems to hit an asymptote as w'/w=2.0. (Figure 10). It can be inferred that as stress concentration increases, the contact area fraction increases.

The results up to this point showed that increasing the tooth length and curving the tooth more towards a python shape caused an increase in the contact area and improved the normal force. The next question we asked was how far the tooth could be loaded without causing injury to the tooth. The mode of failure that was explored was a buckling mode. To estimate the buckling load, a simple 2D model was studied (Figure 5). The load on the tip of this model was increased gradually, and the displacement was tracked. For shorter teeth, buckling was not possible. For longer teeth, buckling was evident by an increase in the lateral and total displacements of the tooth as a function of load.

When these factors were plotted as a function of the parameter w'/w, the point at which buckling became possible was clearly evident. This appeared as a dramatic increase in the total displacement of the tip on the tooth in the finite element results. The critical value of the parameter w'/w at which this occurred was approximately w'/w = 4. The buckling effect comes into consideration, therefore, at a value of the parameter w'/w=4 which is far above the

curvature of a desired tooth shape (Figure 11). Buckling should therefore not be an issue in these designs, and more careful three dimensional buckling analyses that incorporate the stabilizing effect of the tissue were not needed.

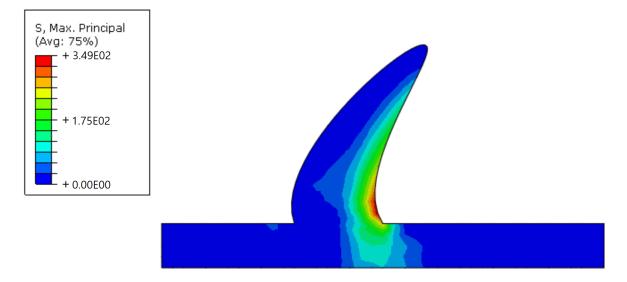


Figure 5. Maximum principal stress contour on tooth model

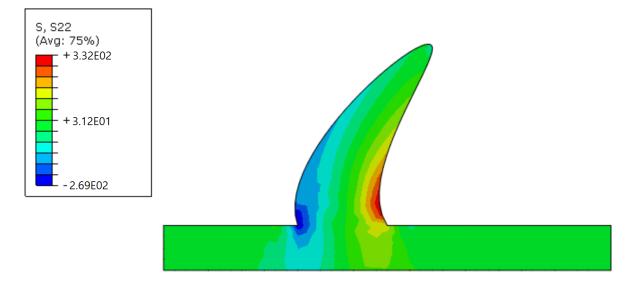


Figure 6. Normal strain in the vertical direction of tooth model

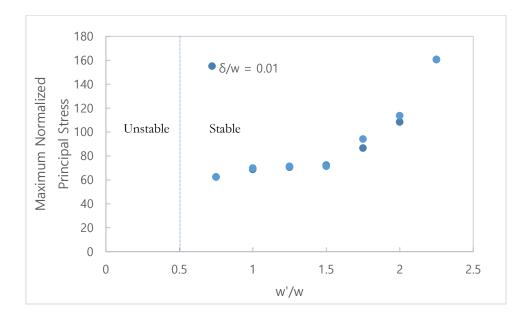


Figure 7. Plot of maximum normalized principal Stress for tendon model

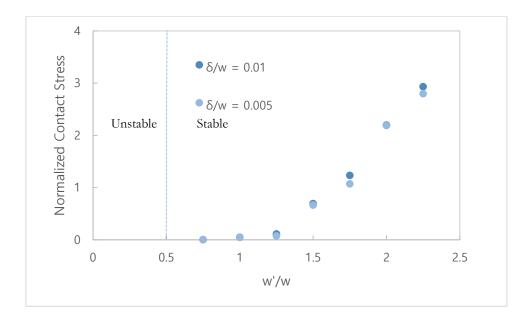


Figure 8. Plot of normalized contact stress for tendon model

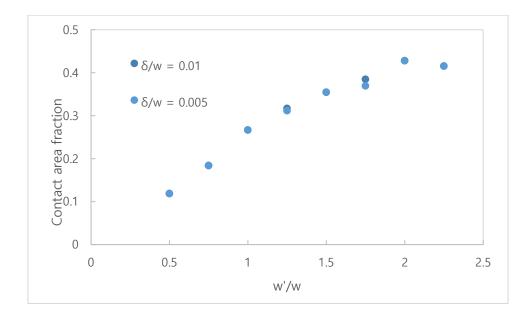


Figure 9. Plot of contact area fraction

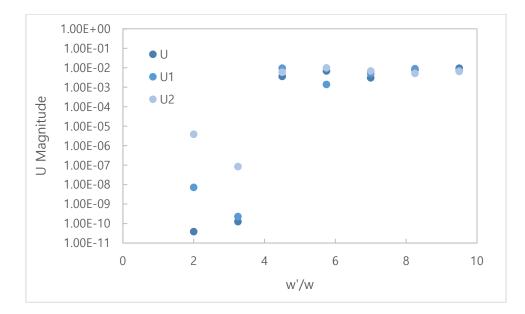


Figure 10. Plot of displacement magnitude of buckling

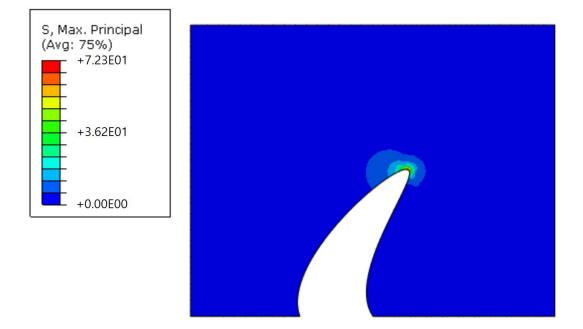


Figure 11. Stress contour of maximum normalized principal stress

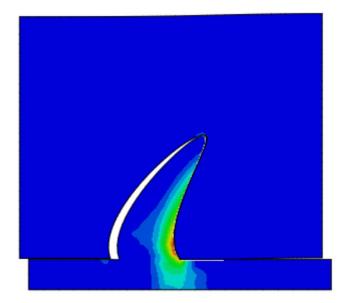


Figure 12. Deformed tendon and tooth model with scale factor of 30

# Chapter 4

## Discussion

A foundation of this study was to start with the simplest possible shape for a tooth, where a simple triangle was subject to a horizontal surface load. The stress values were analyzed and was found that a singularity occurred at the base of the shape. In order to remove this singularity, the next step was to analyze a simple triangle model with a base.

In order to improve the reattachment rate of the human rotator cuff repair, a model resembling a Python tooth was considered. A tooth model with various mesh size and curvatures were analyzed to find an optimal shape. The most important aspects for an optimal shape were to have a firm grip on the tendon, while having low stress values. In order to relieve edge effects, the tooth model was set to penetrate the tendon model until half its total height. As expected the highest region of stress was found to be near the tip area.

The results showed a trend of steady increase in principal stress values as the curvature increased. However, a dramatic increase happened at the curvature point higher than w'/w=1.5. This suggests that the best shape for a tooth is w'/w  $\leq$  1.5 for the purpose of minimizing stress concentrations.

Furthermore, it was seen that as curvature parameter w'/w increased, the contact area fraction increased. The more curved the tooth, the greater the area of tissue that is constrained to be in contact with the gumline due to tooth-tissue interactions. The rate of increase of contact area with respect to tooth curvature decreased around w'/w = 1.5, with a substantial downturn that approached an asymptote (Figure 10).

Finally, the normal stress between the tooth and the gumline increased linearly above w'/w = 1.25. From this perspective, the more curved the tooth the better the vertical constraint. The contact stress was, on average, nearly zero for w'/w  $\leq$  1.25.

Considering the trade-off between these three factors, the optimum shape can be determined to be in the vicinity of w'/w=1.5. This enables a moderate normal force to develop and enables a reasonable fraction of the tissue and gumline to stay in contact, while not substantially increasing the risk of failure associated with higher principal stresses within the tissue.

# Chapter 5

## **Conclusion and Future Directions**

In conclusion, a python tooth model in contact with a tendon model was analyzed. The peak stress values in correspondence with the curvature over displacement time interval data were gathered and plotted. Analyzing the curves, it was found that as the curvature increased, the stress values also increased as well as the contact area. However, the stress values showed an increasing trend as the contact area increased. Considering the trade-off values for contact area, stress values and buckling, the most optimal curvature shape was found to in the vicinity of w'/w = 1.5.

This study introduces an interesting approach to improve the repair rate of the human rotator cuff tear. In future studies, it would be advantageous to research in material mismatches, tooth spacing, and the orthotropy of the tooth shape. The study has many opportunities for further research and would be beneficial to perform more experiments to finalize a product.

A range of simplifying assumptions were made in this study, and future work that relaxes some of these assumptions would be of interest and value. The domain considered for these analyses was meant to mimic an infinitely long array of teeth through the application of periodic boundary conditions. The modeling of isolated teeth near the edge of the tissue would be of interest. The tissue was modeled as isotropic, but many tissues of interest are orthotropic or anisotropic. Modeling the interplay between tissue orthotropy and optimal tooth shape would be another interesting future direction. The specific trade-off between gripping and tearing that various predator teeth make would be interesting to study through application of the approaches developed in this thesis. Finally, it would be interesting to explore these tooth shapes in 3D, and to check how 3D optimization can further define the optimal parameter space.

Despite these assumptions, the thesis establishes that shape optimization can yield a tooth shape that balances the need to avoid tearing flesh with the need to clamp it down to a gumline. The work establishes how an optimized shape might be applied to cinch a tendon-like material to a bone-like material, and lends support to the idea of adapting "teeth" to aid in strengthening and improving the efficacy of tendon-to-bone repairs.

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