Large-Scale Simulation of the Mechanical Response of Porcine Cranial Bone

by

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Submitted to the Department of Aeronautics and Astronautics in partial fulfillment of the requirements for the degree of Master of Science in Aeronautics and Astronautics at the MASSACHUSETTS INSTITUTE OF TECHNOLOGY

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Abstract

Biofidelic computer models are an invaluable tool in the understanding injury biomechanics. One crucial feature of these models is the ability to accurately capture the response of the individual tissues comprising the anatomy under study. In this thesis, we presented a simulation-based approach to describe the stress-strain response of cranial bone in mammals that can be applied to animal studies for model validation purposes as well as in human head injury studies. First, we explicitly characterized a microstructure specimen by generating large biofidelic meshes from μCT images provided by the U.S. Army Research Laboratory (ARL). These meshes capture the intricate structures of the specimen for the model of cranial bone. In addition, different constitutive models were considered to describe the stress-strain response of the constituent cranial bone. Large-scale parallel finite element simulations were conducted and compared to experimental results of uniaxial compression tests of cranial bone of adolescent Göttingen minipigs also conducted at ARL. The experiments show a significant amount of strain localization at different global strain levels, while exhibiting an apparent full elastic recovery upon unloading. Based on the experimental observations, it was found that an elastic hyperfoam model is an excellent candidate for describing the constituent material response. A detailed finite element model using the hyperfoam model for the constituent was able to capture both the stress-strain response and strain localization observed experimentally. The validated full-resolution simulations developed provide the pathway to develop homogenized constitutive models for cranial bone based on microstructural parameters that can be characterized experimentally.

Thesis Supervisor: Raúl Radovitzky
Title: Professor of Aeronautics and Astronautics
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Chapter 1

Introduction

There has been significant interest in recent years in developing biofidelic computer models of the response of the human body to intense mechanical loads, including those resulting from impacts and blasts. The main motivation for the creation of these models is to better understand injuries, which cannot easily be studied by other means (e.g. experimentation on live human subjects) [1–5]. In many such cases, experiments are performed on animal surrogates to gain a better understanding of the injury [6–14]. However, animal studies tend to be limited in quantity, expensive, and the conditions difficult to experimentally replicate for blast impacts. Biofidelic computer models are an invaluable tool that can be used to complement animal studies as they alleviate many of the difficulties associated with experimental studies (i.e. not limited to the number of specimens and the conditions can be consistently applied). Further, the models can lead to a better understanding of injury biomechanics and assist in the development of scaling laws for injuries between animal surrogates and humans [5].

To create a satisfactory computer model of an injury, one key requirement is the inclusion of adequate constitutive models describing the stress-strain response of the individual tissues comprising the anatomy under study, whether it be human or an animal surrogate. However, many current constitutive models in use for biological tissues tend to be inadequate and are incapable of capturing the complex response of the tissues [15] [16].
This thesis is concerned with the development of a simulation-based approach to describe the constitutive response of cranial bone in mammals that can be applied to animal studies for model validation purposes as well as in human head injury studies. The focus is on human head injuries due to their prevalence in the military service members in recent years [17] [18] [19] and in society in general [20]. From 2000-20011, over 235,000 service members, or 4.2% of all who served, were diagnosed with a traumatic brain injury (TBI) and approximately 1.7 million civilians per year in The United States are also diagnosed with TBIs. The work in this thesis accompanies an experimental study conducted by Weerasooriya et al., [21] at the U.S. Army Research Laboratory (ARL) focused on characterizing the mechanical response of small cranial bone specimens extracted from Göttingen minipigs. Those experiments provided a rich data set of both the mechanical response of the specimens and their underlying structure. A brief summary of their experimental results is provided in Chapter 2.

One of the main challenges involved in the modeling of cranial bone is how to incorporate its intricate microstructural details, which determine the global response, into the model. Cranial bone possesses a complex structure that varies by species and with maturity, but even a single cranium can contain vast variations in structural parameters (e.g. porosity & size of trabeculae) depending on the region of the skull and on the depth through the thickness of the skull. Specifically, for adult humans cranial bone takes on sandwich structure composed of a layer of cancellous (spongy) bone in between two layers of cortical bone. However, cranial bone in adolescent Göttingen minipigs varies from compact bone surrounding the brain to cancellous on the exterior surface.

There have been significant efforts to characterize the response of bone tissue documented in literature [22] [23] [24]. Many of the studies have focused on the rate-dependency of bone tissue with McElhaney’s [22] work being one of the oldest to focus on high-strain-rates. His characterization and data are still used today for the validation of potential models. Along with this research, the development of multiple constitutive models for bone tissue has taken place [25] [26] [27]. Of the many potential constitutive models for bone, very
few are capable of capturing the response of bone for the full range of strain-rates occurring for impact loading [28]. Recently, Johnson [26] developed a micromechanics-based model for bone constituent which incorporated elastic, viscoelastic, and inelastic mechanisms of deformation. The model has been shown to accurately capture the response of bone when used as the constituent for both cortical and cancellous bone. Moreover, many of the constitutive models were developed for the constituent, so they ignored micromechanical and spatial-dependency effects associated with cranial bone microstructures. A notable exception is the work performed by Hosseini et al., [29]. They developed a constitutive model of trabecular bone based on both bone volume fraction and trabecular orientation for large compressive strains, and the model has been shown to predict the damage localization and densification of trabecular bone.

In this thesis, we pursue to four step approach to model cranial bone. In the first step, we start by explicitly characterizing the microstructure specimens found in [21] at the microscopic scale for the model. To accomplish this, we will first extract the geometrical information for the specimens’ intricate structures from Micro-Computed Tomography (μCT) images. Using this information, we will then generate large biofidelic meshes for use in finite element models. The details of this procedure is outlined in Chapter 2.

In the second step, we adopt a suitable constitutive model for cranial bone constituent. Several material constitutive models will be examined varying in complexity from a simple linear elastic model to a material model specifically developed to capture the mechanical response of bone tissue. The constitutive models that will be examined in this study are presented in Chapter 3. This process will be assisted by large scale simulations utilizing subsections of the large biofidelic meshes. The idea is these full-resolution microstructure models will enable a one-to-one comparison of the influence of structural variations (e.g. porosity), and they provide a direct comparison to the available experimental data. This process is presented in Chapter 5.

The third step is to validate the full-resolution microstructure models. This will be accom-
plished by first calibrating the chosen constitutive model’s parameters to a single experiment. Using the calibrated parameters, we will then validate the full-resolution models against additional experiments by comparing simulated and experimental responses. During this step, the simulation of each experiment will use a biofidelic mesh generated from the corresponding specimen.

The fourth and final step is to develop a homogenized macroscopic model for cranial bone based on microstructural parameters that can be characterized experimentally. The full-resolution microstructure models incorporating all the structural details through a biofidelic mesh provide a valuable analysis tool, but they have their limitations. Mainly, the level of spatial resolution required to capture the microstructural details is in the order of a few microns and is prohibitive on large sample sizes (e.g. an entire skull). To overcome this limitation, a macroscopic homogenized model is needed that takes the crucial structural information into account through the constitutive model. The shifting of the structural information from the mesh to the constitutive model will drastically reduce the required resolution of the mesh, and would make such a finite element model a valuable tool for full system simulations of injuries.

The far-reaching goal of this study is the creation of a homogenized macroscopic model for cranial bone to assist in the understanding of the mechanics of head injuries. To accomplish this, the model must be usable in system level (i.e. full head) simulations of injury and capture the mechanic response of cranial bone at strain rates ranging from the quasi-static to blast impacts. Such a model could be an invaluable tool in the creation of protective systems and procedures for the prevention and mitigation of head injuries such as traumatic brain injuries.

1.1 Structure of this Thesis

This thesis is organized as follows. This first chapter has established the goals of the study. Next, Chapter 2 will cover the mechanical response and the morphology of the Göttingen
minipig cranial bone that our finite element models will aim to capture. Chapter 3 will continue by discussing the material constitutive models examined in this study. Then Chapter 4 will outline the computational framework used throughout this study. In chapters 5 & 6, we present results from static and dynamic simulations run on the finite element models. Lastly, a discussion and analysis of the behavior of the models are given in Chapter 8.
Chapter 2

Cranial Bone Microstructure Details

There are two important characteristics of the Göttingen minipig cranial bone microstructures that need to be examined to accurately model them: their mechanical response and their morphology. The first section in this chapter will provide a brief explanation of the experiments conducted by Weerasooriya et al., [21], and it will also present the experimental results for specimen MP14002-11. Then the microstructure's morphology will be examined in Section 2.2. Additionally, this section will discuss the process of capturing the specimen's microstructural details in the form of biofidelic meshes.

2.1 Mechanical Response of Cranial Microstructures

Researchers at ARL have been characterizing the mechanical response for cranial bone in adolescent Göttingen minipigs [21]. Their work will assist in the creation of scaling laws for injury between animal surrogates (Göttingen minipigs) and humans in TBI studies. As outlined in [21], a set of specimens have been extracted from three porcine skulls, and they are approximately 4-by-4-mm square sections on the skull surface with the third dimension (depth through the thickness of the skull) varying naturally. A microstructure specimen from their study is shown in Figure 2-1. A subset of the extracted specimens has been tested in a variety of ways (e.g. compression tests, cyclic loading tests).

The study presented in the rest of this paper, however, will focus on a single experi-
Figure 2-1: An extracted cranial bone microstructure from a Göttingen minipig with the average dimensions for the set of remaining specimens use by Weerasooriya et al., [21]

The specific test is an unconfined uniaxial compression test performed on specimen MP14002-11, which has dimensions of 5.19-by-4.68-by-3.46-mm. The experimental setup for this test is outlined in Section 2.1.1 and the mechanical response of the microstructure is described in Section 2.1.2.

2.1.1 Experimental Setup and Procedure

The unconfined uniaxial compression test of MP14002-11 had the microstructure being loaded along the thickness of the skull at a strain rate of $0.001 \text{s}^{-1}$. The setup used by the researchers at ARL is shown in Figure 2-2. A 5kN load cell was used to measure the response of the specimen during the experiment.

Figure 2-2: Experimental setup used by Weerasooriya et al., [21] for compressive loading of cranial bone specimens. The specimens were placed in an Instron servo-hydraulic load frame and loaded while a camera was used to capture the deformation.

In addition to the load cell, ARL used digital image correlation (DIC) to capture the 2D
strain distribution along the thickness of the microstructure. Prior to testing, a side of the specimen was speckled to assist in DIC capturing. During the experiment, a camera (resolution = 1024 x 1024; frame rate = 1 Hz) with a 2X magnification lens was used to capture the deformation in the speckled region of the specimen on which to preform DIC. For correlation on specimen MP14002-11, a subset size of 99px (529 μm) was used, while, the approximate speckle size was 25px (134 μm).

Figure 2-3: The strain computed by DIC for MP14002-11 throughout the uniaxial compression test. The images transition from the undeformed specimen (left) to the strain profile at the end of the experiment (right).

2.1.2 The Mechanical Response of MP14002-11

Based on an analysis of the experimental data received from ARL, a potential model for cranial bone should be able to capture two key features of the results. The first attribute is the stress-strain response, and MP14002-11’s response is shown in Figure 2-4. The experimental stress-strain response begins with a small region of linear behavior (<0.4% Eng strain) followed by a softening in the response between 0.4% and 4% Eng strain. Then, the specimen exhibited a stiffening of its response after 10% Eng strain. In addition, the specimen made an apparent full-elastic recovery upon unloading.

The second attribute a model needs to capture is the strain distribution through the depth of the specimen. Figure 2.1.1 shows the observed strain distributions in MP14002-11 throughout the compression test. From these, experimental strain profiles were created by averaging the strain in each traverse layer along the specimen’s depth, and they are shown in Figures 2-5 and 2-6 for specimen MP14002-11. The experiment shows a significant amount of strain localization in the porous region of the specimen (top surface) at each global strain
Figure 2-4: The mechanical response exhibited by MP14002-11 under unconfined uniaxial compression.

level. This stress-strain response and strain localization are both crucial experimental observations against which simulation results for potential models will be compared.

Figure 2-5: Strain profiles for specimen MP14002-11 at global strain levels of 0-2%. The microstructure exhibited large localization of strain in the porous region of the structure.

2.2 Morphology of the Cranial Microstructures

In addition to understanding the mechanical response of the microstructures, we need to capture the morphology of the specimens to create the full-resolution finite element mod-
Figure 2-6: Strain profiles for specimen MP14002-11 at global strains of 5-15%. The microstructure exhibited large localization of strain in the porous region of the structure.

eels for the specimens. These microstructure specimens are not just homogeneous columns; they have an intricate structure and gradients in their structure. Bone volume fraction (BVF) is one such microstructural parameter with a large variation, and it can be defined as the volume of bone constituent per sample volume. Specifically, cranial bone of Göttingen minipigs exhibits a large gradient in BVF along the depth with little variation in the transverse direction [21], see Figure 2-7. In the region near the brain for specimen MP14002-11, the BVF is around 95%, and the specimen is nearly solid. However, near the outer surface of the skull it has a BVF of approximately 45% and has a porous structure. This can be observed qualitatively by examining an iso-surface of the pores found in MP14002-11, see Figure 2-8. In the figure, the tan color represents the interior surfaces found within the microstructure. Near the top, there are many tiny pores. As expected, there is much more bone material, and when pores are present they tend to be larger in the bottom portion. So, even though the BVF fraction is not 100% in this region the majority of the volume is solid with a few bigger pores resulting in the loss of BVF. In contrast to BVF, the structural orientation of Göttingen minipig cranial bone can be approximated as isotropic at the length scale of the specimens in this study [21]. Finite element models that capture these microstructural characteristics can improve the accuracy of our simulations and analyses, and we accomplished this by generating biofidelic meshes of the microstructure.
Figure 2-7: The bone volume fraction of specimen MP14002-11 calculated from μCT imaging and compared against the bone volume fraction found in the meshes generated from the images. A change from a near solid to a porous structure is present in this specimen.

2.2.1 Image-based Biofidelic Microstructure Meshing

Many imaging methods exist in the biomedical community for the observation of tissue. One prevalent imaging method, Micro-Computed Tomography (μCT), was utilized in this study and many previous studies to generate biofidelic bone geometries from which volumetric meshes of bone specimens were generated. Starting from the raw images, there are a variety of techniques that can be used to create a volumetric finite element mesh. The process we chose to use is outlined briefly below and utilized the software tools Amira [30] and Ansys [31].

The first step of mesh generation procedure is to reconstruct a surface from the images. This is done by loading the images into Amira and applying the Marching Cubes algorithm for 3D surface reconstruction [32] on the images. This results in a triangular surface mesh. The next step is to crop the surface mesh to the desired dimensions. Then, the surface mesh is improved by removing poor quality elements and intersecting surfaces. Amira’s Prepare Tetragen function does most of this automatically, but the last few errors may need to be
Figure 2-8: An iso-surface view of specimen MP14002-11 that highlights the pores found within it. There is an increase in the number of pores present as you move from the bottom to the top of the specimen. The trend in the size of the pores is the reverse.

fixed manually. Finally, the surface geometry is imported into Ansys and a 3D volumetric mesh is generated. If needed, optimization of the 3D mesh can then be performed in Ansys. By following this procedure, high quality biofidelic meshes can be generated.

2.2.2 Meshes for MP14002-11

Using the procedure outlined above, biofidelic meshes for the cranial bone specimen MP14002-11 were generated. μCT images of the specimen with an isotropic voxel size of 2.82 μm was obtained from Dr. Weersooriya’s group at ARL. For the study presented in this paper, a four times resampled set of the original μCT images were used in the mesh generation process. Figures 2-9, 2-10, & 2-11 show surface views and volumetric meshes generated for the specimen. Figure 2-9 shows the mesh for the full microstructure, and the volumetric mesh has 6,347,266 tetrahedral elements. Figure 2-10 shows the mesh for a 1/16th crop of the full microstructures, and the volumetric mesh has 4,361,362 elements. Figure 2-11 shows the mesh for a 1/64th crop of the full specimen, and the volumetric mesh has 886,107
elements. The cropped meshes were generated to reduce the required computation time for each simulation during the process of determining an appropriate constitutive model and calibration of that model. In addition, the crops were taken in such a manner to preserve the structural variation along the depth. As seen in Figure 2-7, the BVF along the depth of the cropped meshes compares well to the experimentally observed values. In the denser portion of the specimen, the meshes' BVFs are slightly higher than the experimental values, but in the porous region they agree well.

Figure 2-9: A one-to-one mesh of specimen MP14002-11 create from a four times resampling of the original μCT data set. The volumetric mesh has 6,347,266 tetrahedral elements
Figure 2-10: A mesh for a $\frac{1}{16}$th subsection of specimen MP14002-11 taken to preserve the structure's variation along the depth. The volumetric mesh has 4,361,362 tetrahedral elements.
Figure 2-11: A mesh for a $\frac{1}{64}$th subsection of specimen MP14002-11 taken to preserve the structure’s variation along the depth. The volumetric mesh has 886,107 tetrahedral elements.
Chapter 3

Modeling the Material Behavior of Cranial Bone

In this study, four potential constitutive model of cranial bone constituent were examined. We looked at a linear elastic model, a neo-Hookean model, a bone model proposed by Johnson et al., [28], and an elastic hyperfoam model. Section 3.1 through Section 3.4 describe the theory for the four material models examined in the study. Justification for the examination of these constitutive models will be provided throughout Chapter 5.

3.1 Linear Elastic Model

The base-line constitutive model examined in this study was an isotropic linear elastic model. The response of this material is expressed in terms of Cauchy stress as

$$\sigma_{ij} = \lambda \epsilon_{kk} \delta_{ij} + 2\mu \epsilon_{ij},$$

(3.1)

where $\lambda$ is the first Lamé parameter, $\mu$ is the second Lamé parameter, and $\epsilon$ is the strain tensor.
3.2 Neo-Hookean Model

The second constitutive model examined was an isotropic non-linear hyperelastic model. Specifically, a neo-Hookean solid model was examined. The Model is defined by the strain energy function

\[ \psi = \frac{\lambda}{2} \ln^2(J) + \frac{\mu}{2} [trC - 3 - 2\ln(J)], \]  

where \( \lambda \) is the first Lamé parameter and \( \mu \) is the second Lamé parameter. Additionally, \( J \) is the Jacobian (the determinant of the deformation gradient) and \( C \) is the Cauchy-Green tensor. This energy function results in a response (in second Piola-Kirchhoff stress) expressed by

\[ S_{IJ} = C^{-1}_{IJ} \ln(J)\lambda + \mu(\delta_{IJ} - C^{-1}_{IJ}). \]  

3.3 Bone Model

The third constitutive model examined by this study was specifically developed for capturing the response of bone. It is a viscoelastic, viscoplastic constitutive model proposed by Johnson et al., [28], and can characterize the response of cortical and trabecular at various strain rates. To accurately capture bone’s viscoelastic behavior, the model incorporates two viscoelastic branches: one low strain rate response and a high rate response. This constitutes a Maxwell-Weichert model with two linear viscoelastic branches. The one-dimensional behavior of this model is given by

\[ \sigma(t) = E_0 \dot{\epsilon}^E t + \eta_1 \dot{\epsilon}^E (1 - e^{-\frac{E_1 t}{\eta_1}}) + \eta_2 \dot{\epsilon}^E (1 - e^{-\frac{E_2 t}{\eta_2}}), \]  

where the superscript VE represents viscoelastic, the subscript 0 refers to the purely elastic branch, and the subscripts 1 & 2 refer to the viscoelastic branches. The viscoplastic component of the model is expressed by the Ramberg-Osgood equation

\[ \dot{\epsilon}^{VP} = \frac{\sigma}{|\sigma|} \left( \frac{|\sigma|}{S_0} \right)^m, \]  

where \( m \) is the inverse of the slope of the trend line between yield stress and strain rate. Ad-
ditionally, the natural logarithm of $S_0$ is given by the y-intercept of the trend line. Finally, the total strain rate of the response is given by

$$
\dot{\epsilon} = \dot{\epsilon}^{VP} + \dot{\epsilon}^{VE}.
$$

A full 3D generalization of this model is given by Johnson et al., [28], and the Summit solid mechanics solver has incorporated it into its constitutive model library.

### 3.4 Ogden Hyperfoam Model

The fourth constitutive model examined in this study was the Ogden hyperfoam model. As describe by Gibson [33], the mechanical behavior of trabecular bone is consistent with cellular materials such as polymeric foams. Three regimes of response under uniaxial compression are exhibited by trabecular bone. First, there is an initial linear elastic response. There is then a plateau of stress from cellular collapse due to elastic buckling, plastic yielding, or brittle fracture. Finally, a region of material stiffening from compaction of the bone is present. This description for the response of trabecular bone is for the overall structural response not for the constituent response. The Ogden hyperfoam model is a purely elastic foam model that is capable of capturing all three of these phases. A constitutive model such as this has potential for use in the homogenized macroscopic model of the response of cranial bone, but it will also be examined as the model for the constituent of the detailed microscopic model.

Additionally, the Ogden hyperfoam model was examined as it offers significant control over its response because users can specify the number of terms in strain energy density function to use, and each term can be calibrated individually. The strain energy function of this model is expressed by

$$
\psi = \sum_{i=1}^{N} \frac{2\mu_i}{\alpha_i^2} \left[ \lambda_1^{\alpha_i} + \lambda_2^{\alpha_i} + \lambda_3^{\alpha_i} - 3 + \frac{1}{\beta_i} (J^{-\alpha_i \beta_i} - 1) \right],
$$

(3.7)
where

$$\beta_i = \frac{\nu_i}{1 - 2\nu_i}, \quad \text{(3.8)}$$

$$J = \lambda_1 \lambda_2 \lambda_3 = \det(F), \quad \text{(3.9)}$$

$$C = \sum_{a=1}^{3} \lambda_a^2 \hat{N}_a \otimes \hat{N}_a. \quad \text{(3.10)}$$

Each term in the series has three variables $\mu_i$, $\nu_i$, and $\alpha_i$, and they represent the shear modulus, Poisson's ratio, and a dimensionless parameter for each term $(i)$ in the series. $\lambda_a$ and $\hat{N}_a$ represent the principal stretches and principal stretch directions, respectively. Additionally, $J$ is the Jacobian and $C$ is the Cauchy-Green tensor. This hyperfoam model is based on the hyperfoam model found in Abaqus [34] with the thermal response removed. The initial shear modulus and bulk modulus of the Ogden hyperfoam model are expressed as

$$\mu_0 = \sum_{i=1}^{N} \mu_i$$

$$K_0 = \sum_{i=1}^{N} 2\mu_i (\frac{1}{3} + \beta_i).$$

The response of a Ogden hyperfoam model (in Second Piola-Kirchhoff stress) is given by Equation 3.11 for three-dimensional finite strain. A full derivation of the stress tensor, material tangent, and celerity of the Ogden hyperfoam model is presented in Appendix A.

$$S_{IJ} = 2 \sum_{i=1}^{N} \frac{\mu_i}{\alpha_i} \left[ \sum_{a=1}^{3} \left( \lambda_a^{\alpha_i - 2} (\hat{N}_a \cdot \hat{e}_I)(\hat{N}_a \cdot \hat{e}_J) \right) - C_{IJ}^{-1} J^{-\alpha_i \beta_i} \right] \quad \text{(3.11)}$$

It should be noted that since bone possess a rate-dependent response [22], this model would only be suitable for a single strain-rate once calibrated since it is a rate-independent model.

### 3.4.1 Implementation in Summit

Steps have been taken to implement the Ogden hyperfoam model into the Summit finite element framework. First, the model's stress tensor, tangent moduli, and celerity were derived...
from its strain energy density function, and this derivation can be found in Appendix A.

Next, a new material was defined within Summit’s material class structure and assigned an identification value at the top level of the material code. Then, the expressions for the stress tensor, tangent moduli, and the celerity were implement into C++ methods in a manner consistent with other material models in Summit. Finally, verification test were performed on this implementation. The tests checked the consistency of the strain energy density function, stresses, and the tangent moduli, and they are outlined in Appendix B.
Chapter 4

Computational Framework

The Summit computational solid mechanics solver was used in this study to model static and dynamic loading. It is a Lagrangian finite element solid solver developed by the Radovitzky group as described in [35] [36], which has a parallel framework implemented in C++. Summit has the capability to use either a continuous Galerkin or a discontinuous Galerkin finite element formulation. In addition, it possesses a wide variety of constitutive models including some specifically developed to describe the response of biological tissues.

4.1 Finite Deformation Numerical Formulation

In the continuum mechanics framework, the deformation gradient tensor \( (F) \) relates displacements in the current configuration to displacements in the reference configuration through the following relation:

\[
F_{ij} = \frac{dx_i}{dX_j}
\]  

(4.1)

In equation 4.1, index \( i \) represents the current finite displacement configuration and index \( I \) represents the reference configuration. The deformation mapping \((\varphi_i(X, t))\) is also a
measure of the current displacement as shown in equation 4.2

\[
F_{ij} = \frac{\partial \varphi_i}{\partial \chi_j} = \frac{dx_i}{dX_j}
\] (4.2)

The ratio of the volume in the current configuration to the volume in the reference configuration is represented by the Jacobian of the deformation \(J\), which is defined as the determinant of the deformation gradient tensor \(J = \det(F)\). The first Piola-Kirchhoff \(P\) stress tensor relates stresses in the current configuration to areas in the undeformed configuration and is expressed by

\[
P_{ij} = J \sigma_{ij} F_{ji}^{-T} = \frac{\partial \psi}{\partial F_{ij}},
\] (4.3)

where \(\sigma\) and \(\psi\) are the Cauchy stress and a strain energy density function, respectively.

Solid mechanics problems are governed by the continuum equation for linear momentum balance, which in its strong form is expressed as

\[
\rho_0 \ddot{\varphi} = \nabla_0 \cdot P + \rho_0 B_0 \in B_0,
\] (4.4)

or in index notation as

\[
\rho_0 \ddot{\varphi}_i = \frac{\partial P_{ij}}{\partial x_j} + \rho_0 B_0 i \in B_0,
\] (4.5)

where \(\rho_0\) is the reference density, \(B_0\) is the body for per unit reference volume, and \(\nabla_0\) is the material gradient operator. For such problems, displacements \(\varphi\) are specified on Dirichlet boundary conditions, and surface tractions \(\bar{T}\) are specified on Neumann boundary conditions, see equations 4.6 - 4.7.

\[
\varphi = \bar{\varphi} \text{ on } \partial_D B_0
\] (4.6)

\[
P \cdot N = \bar{T} \text{ on } \partial_N B_0,
\] (4.7)
with the additional constraints that

\[ \partial_N B_0 \cup \partial_D B_0 = \partial B_0 \]  

(4.8)

\[ \partial_N B_0 \cap \partial_D B_0 = \emptyset, \]  

(4.9)

where \( \partial B_0 \) is the boundary of the body in the reference configuration and \( N \) is the surface normal in the reference configuration.

Next, the weak form of the linear momentum balance integrated in every element and summed over all the elements can be expressed as

\[
\sum_e \left[ \int_{\Omega_e^0} (\rho_0 \delta \varphi_h \cdot \varphi_h + P_h : \nabla_0 \delta \varphi_h) dV - \int_{\partial \Omega_e^0 \cap \partial B_0} \delta \varphi_h \cdot P_h \cdot N dS \right] = 0
\]  

(4.10)

\[
\sum_e \left[ \int_{\Omega_e^0} \rho_0 B \cdot \delta \varphi_h dV + \int_{\partial \Omega_e^0 \cap \partial N B_0} \delta \varphi_h \cdot T dS \right],
\]  

(4.11)

where \( \varphi_h \) is an element-wise continuous polynomial approximation of the deformation mapping and \( \delta \varphi_h \) is the trial function [36]. Additionally, \( \Omega_e^0 \) and \( \partial \Omega_e^0 \) are the domain and boundary of the domain for element \( e \), respectively.

For the analysis in this thesis, only Summit's continuous Galerkin (CG) finite element formulation was used. The CG weak form is shown in Equation 4.12, and is the result of enforcing continuity of displacements between elements on Equation 4.10.

\[
\sum_e \left[ \int_{\Omega_e^0} (\rho_0 \delta \varphi_h \cdot \varphi_h + P_h : \nabla_0 \delta \varphi_h) dV \right] = \sum_e \left[ \int_{\Omega_e^0} \rho_0 B \cdot \delta \varphi_h dV + \int_{\partial \Omega_e^0 \cap \partial N B_0} \delta \varphi_h \cdot T dS \right]
\]  

(4.12)
4.2 Solvers

The analyses performed in this paper utilized two solvers: one static and one dynamic. The static solver was a nonlinear conjugate gradient method [37], and its details are outlined in Section 4.2.1. The dynamic solver was the Newmark-beta method implemented in Summit, and it is discussed more in Section 4.2.2.

4.2.1 Solver: Nonlinear Conjugate Gradient

The Portable, Extensible Toolkit for Scientific Computation (PETSc) is a suite of data structures and routines for scalable solutions to problems modeled by partial differential equations [38]. Summit includes interfaces to many of PETSc's algorithms for solving linear and nonlinear systems. In Summit, the algorithms are used to solve the boundary value problem outlined in Section 4.1. For the work presented in this thesis, PETSc's nonlinear conjugate gradient method based on residuals was chosen as the static solver because it included many desirable features including scalability to a large number of processors. It is part of PETSc's SNES package, and an interface to the method was provided by Summit's PetscNCG solver class. The remainder of this section will outline both our choice of preconditioner and convergence criteria, and demonstrate the scalability of the PetscNCG solver class.

Two preconditioners were considered for use in our analyses: a mass and Jacobi preconditioner. These are both simple preconditioners; however, based on the problem in question their performance can differ dramatically. For example, a simulation of a single compressive load step was run using each of the preconditioners on an uniform and nonuniform mesh, which are shown in Figures 4-1a & 4-2a, respectively. Additionally, they were tested with both a linear (i.e. linear elastic) and nonlinear (i.e. Ogden hyperfoam) material model. The performances of the two preconditioners are comparable for a uniform mesh (See Figures 4-1b & 4-1c), but the Jacobi preconditioner performed substantially better than the mass preconditioner for the nonuniform mesh (See Figures 4-2b & 4-2c). For the case of a linear material model and the nonuniform mesh, both solutions converged, but the
simulation utilizing the Jacobi preconditioner converged in 2372 less iterations. With a nonlinear material model and a nonuniform mesh, only the simulation utilizing the Jacobi preconditioner converged. The solution for the simulation utilizing the mass preconditioner diverged, and the simulation failed. The biofidelic meshes for cranial bone that were used in this study are nonuniform meshes; therefore, the Jacobi preconditioner was used for all the static simulations presented in the rest of the study because it was shown to perform better on nonuniform meshes.

Further, we examined the choice of convergence criterion for a simulation running on a
nonuniform mesh. The PetscNCG solver class has set the convergence criterion of the iterative static solver to be the relative tolerance of the residual, but the choice of the norm used in the comparison can be specified. A comparison of the performance of $L_\infty$ and $L_2$ norms, two commonly used norms, of the residual can be seen in Figure 4-3. The results of the study show little difference in the choice of norm used to determine convergence; however, the $L_2$ norm of the residual is marginally higher than that of the $L_\infty$ norm at the end of the simulation. Of the two norms, the $L_2$ norm seems to provide the worst case scenario in the remaining residuals in the system, and it was chosen as the convergence criterion. By choosing the $L_2$ norm, additional iterations (compared to the iterations for the $L_\infty$ norm) will be performed by the solver to reach convergence, which should result in a slightly more accurate solution.

![Figure 4-3: Comparison of $L_\infty$ and $L_2$ Convergence](image)

In addition, a key feature of both Summit and PETSc is the ability to scalably solve problems, and interfacing between the two libraries needs to preserve this feature. A small study of Summit’s PetscNCG solver class was performed to ensure that the scalability remained. A single load step simulation was run on meshes with 253,395, 1,161,070, and 1,718,170 degrees of freedom (dofs) in parallel with an increasing number of processors (1, 2, 4, 8, 16, 32, 64, 128, 200, & 232). The required computation time was measured for each combination of dofs and number of processors. The results of this study show strong scalability of Summit’s PetscNCG solver, see Figure 4-4. The decrease in computation time for
the mesh with the least dofs appears to flatten out when the simulation was run on a large number of processors, but that is to be expected as communication time begins to dominate.

![Diagram](image)

**Figure 4-4:** Strong scalability of the interfaced PETSc solver found in Summit.

In summary, the quasi-static analyses described in this thesis used Summit’s PetscNCG solver which is interfaced to PETSc’s nonlinear conjugate gradient method in a manner that retains it’s scalability. The solver used a Jacobi preconditioner and convergence was determined by comparing the relative tolerance of the $L_2$ norm of the problems residual.

### 4.2.2 Solver: Newark Scheme

To solve the structural dynamics problem, a Newmark time stepping algorithm is available in Summit. The algorithm is expressed by Equations 4.13 - 4.15. In Summit, the Newmark parameters ($\gamma$ and $\beta$) are set to 0 and 0.5, respectively.

\[
x_i^{n+1} = x_i^n + \Delta t \ddot{x}_i^n + \Delta t^2 \left( \frac{1}{2} \right) \dddot{x}_i^n + \beta \dddot{x}_i^{n+1}
\]  

(4.13)

\[
\ddot{x}_i^{n+1} = \ddot{x}_i^n + \Delta t \left( (1 - \gamma) \dddot{x}_i^n + \gamma \dddot{x}_i^{n+1} \right)
\]  

(4.14)

\[
\dddot{x}_i^{n+1} = M_i^{-1} \left[ f_i^{ext} - f_i^{int} \right]^{n+1}_j
\]  

(4.15)
The variables $M$, $f_{ext}$, and $f_{int}$ found in Equations 4.13 - 4.15 are a lumped mass matrix, the external force on the system, and the internal force in the system, respectively. The subscript $i$ represents the spatial discretization and the subscript $n$ is the temporal discretization.
Chapter 5

Quasi-static Simulations

In this chapter, an examination of both the detailed finite element model and a proposed homogenized macroscopic finite element model for cranial bone is provided. For the detailed finite element model, full-resolution static simulations were conducted to evaluate four potential models for the constituent of Göttingen cranial bone. A static simulation was also conducted on the proposed homogenized macroscopic model to evaluate its ability to capture the experimental response Göttingen cranial bone. Specifically, all the models were evaluated on their ability to capture both the stress-strain response and strain localization experimentally observed in specimen MP14002-11.

This chapter is organized in the following way. Section 5.1 describes the setup used to simulated ARL’s experiments on cranial bone specimens. Next, Section 5.2 describes the post-processing technique used to generate simulated strain profiles for comparison to the experimental profiles. Sections 5.3-5.6 each provide the results of a simulations for the detailed finite element model with one of the potential constitutive models. Section 5.7 then examines and discusses a first attempt at a homogenized macroscopic model of cranial bone. Finally, an evaluation of the models are provide in Section 5.8.
5.1 Simulation Setup

To simulate the quasi-static experiments performed by ARL, a Summit static simulation driver was set up for an unconfined uniaxial compression test. The boundary conditions applied were as follows: a roller placed on one x face, a roller placed on one y face, a roller on the bottom z face, and a roller on the top z face that is incrementally displaced to a user specified strain level. A schematic of the boundary conditions is shown in Figure 5.1. Summit’s PetscNCG solver was used in the simulation driver. This simulation setup was used for the examination and analyses of both the detailed finite element model and the homogenized macroscopic model in this chapter. A biofidelic mesh was used in the full-resolution simulations of the detail finite element model, and a solid column mesh was used in the simulation of the homogenized macroscopic model.

![Schematic of boundary conditions](image)

Figure 5-1: Schematic of boundary conditions applied to microstructures during the static simulations.

5.2 Post-processing of Simulation Data

One of the key tools used to record experimental results for ARL’s study of Göttingen minipig cranial bone was digital image correlation. DIC is based on optically tracking the
location of points on the specimen and comparing them to the locations at previous time steps to compute displacement. Deformation is then computed from the displacements. For the experiment conducted on MP14002-11, DIC was performed on a single face of the specimen, and the experimental strain profiles were generated from the collected DIC data.

In this study, strain profile of the simulated strain localization were generated by using a post-processing procedure based on the finite difference method for comparison to the experimental profiles. This procedure was chosen to mimic the DIC procedure, and it computes strain in the specimen based on displacements. The post-processing procedure is outlined below.

After a simulation was complete, the mesh was divided into N subsections along the depth, see Figure 5.2. The average displacement \( u_3 \) in the direction of the depth (subscript 3 in Summit’s notation) and the location \( x_3 \) of center of the section were computed for each subsection \( (i=1 \text{ to } N) \). Then, the 2nd-Order Central Difference method defined in Equation 5.1 was applied to compute the normal strain along the loading direction \( \epsilon_{33} \) in each subsection. Finally, these linearized strains were used to generate the strain profiles of the simulated strain localization.

\[
\epsilon_{33}^i = \frac{u_3^{i+1} - u_3^{i-1}}{2(x_3^i - x_3^{i-1})}
\]

(5.1)

For many simulations, this additional post-processing procedure would not be necessary, and simply averaging the simulation’s strain at each level would be sufficient for the generation of strain profiles. However, this is not the case for the simulations using the complex biofidelic meshes of cranial bone. As an example, consider the simulated strain along the depth present in the microstructure shown in Figure 5-3. It shows the simulated strains in a microstructure compressed to 10% engineering strain using the linear elastic material model. In this simulation, there were a few small areas in the vertical pillars where the strain was localized and collapse occurred. In contrast to these small regions, there were
Figure 5-2: A schematic of the proposed finite difference method to compute the strain found in the microstructure simulations.

Figure 5-3: Strain localization in a microstructure simulation use a linear elastic material model. In this simulation, the vertical columns in the microstructure contain almost all of the strain. The regions away from the vertical columns have nearly zero strain. Thus, purely averaging the strain in the microstructure would not provide an accurate account of the deformation along its depth as compared to the results observed by DIC.
comparatively large regions with near zero strain in the direction of the depth. These regions were still displaced due to the collapse of the vertical pillars, but experienced little strain themselves.

Figure 5-4: Comparison of the strain profiles generated by averaging strain and the proposed DIC mimicking procedure. The DIC mimicking procedure produces a greater localization of strain in the porous region compared to purely averaging the strain for the same microstructure simulation.

For this simulation, a comparison of the two strain profile generating procedures is shown in Figure 5-4, and the strain profiles generated by the two procedures differ dramatically. Averaging the strain resulted in a strain profile that was nearly flat, whereas the finite difference post-processing procedure produced a curve with a large amount of strain localization in the porous region. For a microstructure simulation, generation of strain profiles by averaging the strains at each level creates profiles that are skewed by the microscopic regions of low strain and that miss the strains observed at the macroscopic level.

In addition to this simple example, the use of a nonlinear material model can produce another complication through buckling. Under compression, the trabeculae of a microstructure can buckle, and this mechanism leads to regions of local tension within the trabeculae. Just as with the regions of low strain, these microscopic regions of tension skew the strain profiles generated by simply averaging the strain.
Neither of these microscopic regions are taken into account by DIC because it is based on macroscopic displacement. Thus, the experimental strain profiles do not compare effectively to strain profiles created by averaging the simulated strain at each layer through the depth of the microstructure. However, the simulated strain profiles generate by the post-processing procedure we used do compare effectively against the experimental profiles because they both compute strain from displacement.

### Table 5.1: Linear Elastic Constitutive Parameters

<table>
<thead>
<tr>
<th>$\rho$ ($kg/m^3$)</th>
<th>$E$ (Pa)</th>
<th>$\nu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1810</td>
<td>$3.1 \times 10^9$</td>
<td>0.22</td>
</tr>
</tbody>
</table>

5.3 **Linear elastic Simulation Results**

The first model examined as the constituent for the detailed finite element model was the isotropic linear elastic model. The examination was completed by using the simulation setup outlined in Section 5.1 and the post-processing procedure outlined in Section 5.2. The compression simulation was run to 15% engineering strain with the $\frac{1}{64}$th subsection mesh of MP14022-11 with 886 thousand elements. A single set of material constants was set for the entire mesh, and the parameters can be seen in Table 5.1. Using a single set of material parameters for the entire microstructure allow an examination of the effects of the specimen’s porosity. The Young’s modulus used in the simulation was chosen to match the bone specimen’s Young’s modulus for the material with no pores.

Figure 5-5 shows the simulated stress-strain response compared to the experimental response. The simulated response diverges from the experimental response after approximately 0.4% strain. This indicates that a more complicated material model will be needed to capture the response of the cranial bone microstructures. The presence of the pores in the microstructure resulted in a response that was $\sim 59\%$ less stiff than the inputted Young’s modulus.
Figure 5-5: Comparison of the simulated mechanical response using a linear elastic material model to the experimental mechanical response for MP14002-11. The simulation used a mesh that was a \( \frac{1}{64} \) subsection of the total specimen.

Additionally, the simulated strain profiles are shown in Figures 5-6 & 5-7. For the small global strains (0% - 2%), the simulation failed to capture the localization of strain in the porous region. This implies that an appropriate material model needs to accommodate more strain at the same level of stress. Again, this result indicates that a more complex model of the constituent is required to accurately model cranial bone.

Figure 5-6: Comparison of simulated and experimental strain profiles for a linear elastic material model - small strain levels.
Figure 5-7: Comparison of simulated and experimental strain profiles for a linear elastic material model - intermediate strain levels.

<table>
<thead>
<tr>
<th>$\rho \left( \frac{kg}{m^3} \right)$</th>
<th>$E$ (Pa)</th>
<th>$\nu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1810</td>
<td>$3.1 \times 10^9$</td>
<td>0.22</td>
</tr>
</tbody>
</table>

Table 5.2: NeoHookean Constitutive Parameters

Based on both of these results, a detailed finite element model with the linear elastic model for the constituent is insufficient to capture the response of Göttingen minipig cranial bone.

5.4 Neo-Hookean Simulation Results

The next constitutive model examined in the detailed finite element model was Summit’s neo-Hookean model extended to the compressible range. The linear elastic material was unable to capture either the softening in the response or the localized strain in the porous regions, so we turned to a nonlinear elastic model. This was done because the use of compressible hyperelastic models, which lead to nonlinear geometric effects (i.e. buckling), in simulations of foam like structures have been shown to produce a softening in the stress-strain response [39].

Again, the detail finite element model was examined by conducting a uniaxial compression simulation up to 15% engineering strain. The neo-Hookean model parameters used were
the same as those used with the linear elastic model, and they are shown in Table 5.2. They are the same because in the small strain region, the linear elastic and neo-Hookean models have the same response. The effects of the neo-Hookean model should be seen at higher strain levels. In addition, the simulation of the experiment used the $\frac{1}{64}$th subsection mesh of MP14022-11 with 886 thousand elements.

Figure 5.4 shows the simulated stress-strain response of MP14002-11 using the neo-Hookean material model compared to the experimental response. Again, in the region of strain under 0.5%, the simulated response agrees with the experimental results. However, the two results soon diverge. In this simulation, softening in the stress-strain was observed after 6% strain. This simulated softening, however, is minimal in comparison to what occurred experimentally. Additionally, the simulated softening begins at a strain level almost 5.5% higher than the onset in the experiment.

![Figure 5.4](image)

(a) Small Strain Response  
(b) Overall Response

Figure 5-8: Comparison of the simulated mechanical response using a neo-Hookean material model to the experimental mechanical response for MP14002-11. The simulation used a mesh that was a $\frac{1}{64}$th subsection of the total specimen.

Once again, there was a little localization of strain in the porous region, but not enough to match the localization exhibited by MP14002-11 in the small strain range of the experiment (See Figures 5-9 & 5-10). Under the assumption that our meshing procedure accurately captured MP14002-11’s structure, the nonlinear geometric effects seem to be minimal and
Figure 5-9: Comparison of simulated and experimental strain profiles for a neo-Hookean material model - small strain levels.

Figure 5-10: Comparison of simulated and experimental strain profiles for a neo-Hookean material model - intermediate strain levels.
not likely the single mechanism causing the softening in the response and strain localization. Therefore, a more complex constitutive law is required to capture the response of porcine cranial bone. The model for the constituent should accommodate more strain at the same level of stress than either the simulated responses for the linear elastic or neo-Hookean model. This means that at a constitutive level, a nonlinear response which softens under compressive loading is required to capture the global response for the microstructure.

### 5.5 Bone Model Simulation Results

In consideration of the need for a softening in the response of the constitutive material, Johnson’s constitutive model for bone was examined as a potential model for the constituent in the detailed finite element model. The softening of this model’s response is due to plasticity. Shown in Table 5.3 are the constitutive parameters that were used in this study. Calibration of the parameters was accomplished by successively performing simulations and sweeping the parameter values. Only the parameters \( E_0 \), \( S_0 \), \( m \) were considered during calibration because the simulations were conducted at a quasi-static strain rate, and the viscoelastic branches contribute a minimal stress response at quasi-static rates. Furthermore, \( E_0 \) required little calibration because it corresponds to the purely elastic branch of the model, and it only required a small variation from the value used for the linear elastic and neo-Hookean models.

<table>
<thead>
<tr>
<th>( E_0 ) (Pa)</th>
<th>( E_1 ) (Pa)</th>
<th>( E_2 ) (Pa)</th>
<th>( \eta_1 ) (Pa s)</th>
<th>( \eta_2 ) (Pa s)</th>
<th>( \nu )</th>
<th>( S_0 ) (Pa)</th>
<th>( m )</th>
<th>( \rho \left( \frac{kg}{m^2} \right) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 3.08 \times 10^9 )</td>
<td>( 2.5 \times 10^7 )</td>
<td>( 2.5 \times 10^7 )</td>
<td>( 128 \times 10^6 )</td>
<td>( 8.2 \times 10^4 )</td>
<td>0.36</td>
<td>( 45.6 \times 10^6 )</td>
<td>18.10</td>
<td>1810</td>
</tr>
</tbody>
</table>

Table 5.3: Constitutive Parameters for Johnson’s Bone Model

The simulated small strain response for MP14002-11 using Johnson’s bone model is shown in Figure 5-11. With the chosen parameters, enough softening in the simulated response was exhibited by the microstructure. In fact, too much softening in the response occurred, and the simulated response begins to undershoot the experimental response after 0.6% en-
engineering strain.

![Figure 5-11: Comparison of the simulated mechanical response using Johnson's material model for bone to the experimental mechanical response for MP14002-11. The simulation used a mesh that was a $\frac{1}{64}$ subsection of the total specimen.](image)

With this constitutive model, the desired localization of strain in the porous region is also achieved, as shown in Figure 5-12. In fact, for the strain level of 1.5%, there is a greater localization of strain in the porous region in the simulation than was observed experimentally.

Before this model could be fully calibrated, we were informed that the specimen made an apparent full elastic recovery (i.e. no plastic deformation) from the compression test. Thus, the mechanism from the bone constitutive model resulting in the softening is not applicable. However, this model does capture the response of MP14002-11 well, and even better results could be obtained with a more precise calibration of the model. It should be noted that in previous studies of trabecular bone, the softening of its response has been attributed to plastic mechanisms [40] [41]. So, if plasticity is either observed in the other specimens in ARL’s study or is determined to be a contributing factor to the softening in this specimens response, Johnson’s bone model could still be a potential model for the constituent of Göttingen minipig cranial bone.
Figure 5-12: Comparison of simulated and experimental strain profiles for Johnson's material model for bone - small strain levels.

5.6 Hyperfoam Simulation Results

The final model that was examined for the constituent in the detailed microscopic finite element model was the Ogden Hyperfoam model. This model was chosen because at a constitutive level it exhibits a plateau in its stress response under compressive loading, and the softening is due to purely elastic mechanisms. The results shown below are from a simulation using only a single term in the series of the strain energy density function for the model, and the calibrated parameters are shown in Table 5.4. Since the use of Johnson's bone model produced a desirable stress-strain response and strain profiles, we used it as a base in the calibration process of the parameters for the Ogden hyperfoam. The idea was to avoid a full calibration process, which would have required running simulations with the microstructure mesh. Specifically, the 1D analytical uniaxial stress-stretch relation (Equation 5.2) for the Ogden hyperfoam model was matched to the bone model's known 1D uniaxial constituent response to determine the parameters for the hyperfoam model.

\[ P_{33} = \frac{2}{\lambda_3} \sum_{i=1}^{N} \frac{\mu_i}{\alpha_i} (\lambda_3^{\gamma_i} - J^{-\alpha_i \delta_i}) \]  

(5.2)

Shown in Figure 5-13 is the simulated response of specimen MP14002-11 with the Ogden hyperfoam as the constitutive model. The simulated response accurately captured the ex-
Table 5.4: Ogden Hyperfoam Constitutive Parameters

<table>
<thead>
<tr>
<th></th>
<th>ρ (kg/m³)</th>
<th>N</th>
<th>μ₁ (Pa)</th>
<th>ν₁</th>
<th>α₁</th>
</tr>
</thead>
<tbody>
<tr>
<td>1810</td>
<td>1</td>
<td>2 x 10⁹</td>
<td>0.03</td>
<td>100</td>
<td></td>
</tr>
</tbody>
</table>

Experimental response in the small strain region (0-2%). The two response start to diverge after 5% strain, but they remain relatively close. With the addition of a second term in the series or additional calibration of the parameters to the high strain regions this model should be able to capture the experimental response of MP14002-11 over the entire experimental range.

Figure 5-13: Comparison of the simulated mechanical response using Ogden hyperfoam material model to the experimental mechanical response for MP14002-11. The simulation used a mesh that was a 1/64th subsection of the total specimen.

In addition to capturing the stress response of the specimen, this constitutive model also does a good job at capturing the strain localization in the specimen, as shown in Figures 5-14 & 5-15. The simulated strain profiles fit well for all the strain profiles except at 15% Eng strain. One possible explanation is that at 15% strain the experimental and simulated stress-strain responses are the farthest apart, and the simulated response is lower than the experimental response for this strain level. This could result in the extra strain localization exhibited by the simulated response.

Overall, the Ogden hyperfoam material in conjunction with the biofidelic mesh of MP14002-
Figure 5-14: Comparison of simulated and experimental strain profiles for the Ogden hyperfoam material model - small strain levels.

Figure 5-15: Comparison of simulated and experimental strain profiles for the Ogden hyperfoam material model - intermediate strain levels.
11 appears to be an excellent candidate for a detailed microscopic finite element model of the cranial bone of Göttingen minipigs. It currently captures the stress-strain response over a range of 0-5% strain. Additionally, the model reproduces the strain localization in the porous region through an elastic mechanism. Finally, the model could provide even closer results with the inclusion of another term from the strain energy function or with more calibration to the higher strain level data.

5.7 Parametric Linear Elastic Simulation Results

In addition to the microscopic model for the cranial bone, a basic homogenized model proposed by ARL was examined for the specimen. In the models shown above, a single set of material parameters was used for the entire structure and a biofidelic mesh was used to capture the geometry. However, the proposed homogenized macroscopic model will use a monolithic mesh (See Figure 5-17a) and vary the material parameters through its depth. As a first attempt to characterize the response of the cranial bone, ARL using DIC split the specimen into 10 sections along the depth and fit an elastic modulus for each region, see Figure 5-16.

Using their values, a quadratic fit was generated for the elastic modulus through the depth of the specimen, see Figure 5-17b. This expression was passed into a simulation using a parametric linear elastic material and the monolithic mesh. The simulated mechanical response of this simulation is shown in Figure 5-18, and it doesn’t capture the experimental stress-strain response in either the small or intermediate strain ranges.

Additionally, the simulated strain profiles for the homogenized macroscopic model are shown in Figures 5-19 & 5-20. The model captures the localization of strain in the porous region for small strains, but at the intermediate strain levels the localization is too great. A drawback of using a linear elastic model is that the shape of the profiles won’t change based on the global strain levels. The curves will only be scaled based on them.
Figure 5-16: ARL's fit of an elastic modulus to each section through the depth of specimen MP14002-11.

(a) Macroscopic Mesh

(b) The quadratic fit to the experimental elastic moduli values used in homogenized model

Figure 5-17: Setup of the homogenized macroscopic model
Figure 5-18: Comparison of the simulated mechanical response of the homogenized linear elastic model to the experimental mechanical response for MP14002-11.

Figure 5-19: Comparison of simulated and experimental strain profiles for the homogenized linear elastic model - small strain levels.
Figure 5-20: Comparison of simulated and experimental strain profiles for the homogenized linear elastic model - intermediate strain levels.

Based on the simulated stress-strain response and strain profiles, a homogenized macroscopic model based on linear elasticity is insufficient to capture the response of cranial bone in Göttingen minipigs. The examination of more complex homogenized models is required to better capture the response of the cranial bone.

5.8 Discussion

Two conclusions have been drawn from the analyses of the static simulations presented in this Chapter. First, the Ogden hyperfoam model is an excellent candidate for the constituent in the detailed microscopic finite element model of Göttingen minipig cranial bone. Four constitutive models were examined, and the Ogden hyperfoam model was determined to be the most appropriate. The detailed finite element model using a biofidelic mesh and the Ogden hyperfoam model as its constitutive model captured both the stress-strain response and the strain localization experimentally exhibited by specimen MP14002-11. Further, this constitutive model is purely elastic, so it would be able to recover after compression as the specimen did after the uniaxial experiment.

Second, a macroscopic homogenized finite element model based on a linear elastic material
model with varying elastic modulus along the depth is insufficient to model Göttingen minipig cranial bone. A more sophisticated macroscopic model is required to capture the strain localization and the mechanical response.
Chapter 6

Dynamic Simulations

A long term goal of this research is to model cranial bone at a variety of strain rates. This includes the high strain rates that correspond to blast impacts. Up to this point, we have only analyzed and tried to model experiments performed at a quasi-static strain rate. To model experiments that occur at rates faster than the quasi-static, dynamic simulations are required. A Summit dynamic simulation driver has been setup for a uniaxial compression test, and the setup is given in Section 6.1. In the absence of experimental results at rates other than quasi-static, this work was primarily completed in preparation for future high strain rate data to be used in the modeling process.

Section 6.2 presents the results of several simulations conducted to test the driver setup. The simulations were performed on a set of five microstructure meshes provided by Dr. Kraft of the Pennsylvania State University. These meshes (200-500 thousand tetrahedral elements) have fewer elements than the large biofidelic meshes for specimen MP14002-11.

6.1 Dynamic Simulation Setup

A Summit dynamic simulation driver was setup for an unconfined uniaxial compression test. The driver used Summit’s ExplicitNewmarkIntegratorLumpMass, which uses the explicit Newmark time integration scheme to solve the structural dynamics problem. The boundary conditions were as follows: a roller on the bottom z face, and a roller on the top
Figure 6-1: Microstructure data set provided by Dr. Kraft of the Pennsylvania State University used to test the dynamic driver.

<table>
<thead>
<tr>
<th>( \rho , (\text{kg/m}^3) )</th>
<th>( E , (\text{Pa}) )</th>
<th>( \nu )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1810</td>
<td>2.0 \times 10^{10}</td>
<td>0.22</td>
</tr>
</tbody>
</table>

Table 6.1: Neo-Hookean constitutive parameters for the dynamic simulations

A face that is incrementally displaced at a user specified strain rate. A schematic of the boundary conditions is shown in Figure 6.1.

### 6.2 Dynamic Simulation Results

The dynamic driver was tested by running a series of simulations modeling a uniaxial compression test at a strain rate of 1000 s\(^{-1}\). The simulations were run with the five meshes shown in Figure 6-1 and two material models: a rate independent and a rate dependent model. The rate independent model was Summit’s neo-Hookean model and the rate de-

<table>
<thead>
<tr>
<th>( E_0 , (\text{Pa}) )</th>
<th>( E_1 , (\text{Pa}) )</th>
<th>( E_2 , (\text{Pa}) )</th>
<th>( \eta_1 , (\text{Pa} , \text{s}) )</th>
<th>( \eta_2 , (\text{Pa} , \text{s}) )</th>
<th>( \nu )</th>
<th>( S_0 , (\text{Pa}) )</th>
<th>( m )</th>
<th>( \rho , (\text{kg/m}^3) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.62 \times 10^{10}</td>
<td>4.4 \times 10^{9}</td>
<td>2.36 \times 10^{10}</td>
<td>1.325 \times 10^{8}</td>
<td>0.2268 \times 10^{8}</td>
<td>0.36</td>
<td>2.22 \times 10^{8}</td>
<td>18.24</td>
<td>1810</td>
</tr>
</tbody>
</table>

Table 6.2: Constitutive parameters for Johnson’s bone model for the dynamic simulations
The independent model was the constitutive model for bone developed by Johnson et al., [28]. The constitutive parameters used for the two models can be found in Tables 6.1 & 6.2.

The simulated responses of the microstructures are shown in Figures 6-3 & 6-4. The microstructure meshes vary in BVF from 76-91%, and their responses are compared against the simulated dynamic response of a solid (100% BVF) cube. Based on the simulated stress-strain responses, average bone volume fraction of a microstructure does not directly correspond to simulated stiffness. In fact, Microstructure 1, which had the second highest BVF, had the lowest simulated stiffness of all the microstructures.

6.3 Discussion

While these simulated results were not directly comparable to any experimental results, they were insightful. Two major insights came from setting up and running a set of dynamic simulations. First, high average BVF of a microstructure does not necessarily correspond to highly stiff response of the microstructure. The morphology of the bone leading to a specific BVF appears to play a significant role in the stiffness of the response. This
Figure 6-3: Dynamic Response of the microstructures provided by Dr. Kraft.

Figure 6-4: Dynamic response of the microstructures provided by Dr. Kraft. (Green) Neo-Hookean average response with 95% confidence interval. (Blue) Johnson's bone model average response with 95% confidence interval.
information will be useful during the future development of a homogenized macroscopic model for the response of cranial bone.

Second, we learned the required computation time for a dynamic simulation using a biofidelic mesh of a microstructure at low strain rates is prohibitive. Microstructure simulations with strain rates below approximately 100s$^{-1}$ were unmanageable without tools to decrease the required computational time. One potential tool to decrease a dynamic simulation’s computation time is mass scaling, which will be discussed in Chapter 7.
Chapter 7

Mass Scaling

Mass scaling is a computational tool to reduce the computation time of a dynamical simulation with little alteration to its final results by increasing the simulation’s critical time step [42]. The addition of artificial mass into the simulation is responsible for the increased time step, leading to the tool's name. Implementation of mass scaling, in some form, can be found in numerous commercial finite element packages including Abaqus [34] and LS-DYNA [43] because it can provide this crucial reduction in computation time. Small critical time steps for a simulation can arise from a variety of reasons, but two specific scenarios have presented themselves through the simulation of cranial bone specimens. Further, both scenarios are good candidates for applying mass scaling.

The first case was when only a few poorly conditioned elements led to a low critical time step at the beginning of the simulation. This occurred mainly due to the desire to preserve geometric integrity during mesh generation, and when mesh generation was outside of our control.

The second case was when elements collapsed during the simulation and dragged down the critical time step. For microstructure meshes, there can be strain localization leading to element collapse even at relatively low global strains. This collapse sharply decreases the critical time step of dynamic simulations as shown in Figure 7-1. If the critical time step decrease is great enough, it stalls the simulation. The critical time step profile that is
shown in Figure 7-1 is from a simulation on a microstructure that stalled for this reason. With a final critical time step of $1 \times 10^{-19}$ s, the time required to make meaningful progress became unreasonable, and the simulation was terminated.

![Critical Time Step of Simulation with Element Collapse](image)

Figure 7-1: The decrease in the critical time step of a dynamic simulation due to the collapse of an element. This drastic decrease in the critical time step leads to the stalling of the simulation.

For this particular study, these two cases are not entirely independent of each other. In general, this does not necessarily have to be true. To resolve the issue of the small critical time step in each case, the application of mass scaling should differ slightly. For the first case, mass scaling can be used to remove the effects of the few poorly conditioned elements and set the critical time step closer to that of the better conditioned elements once at the beginning of the simulation. In the second case, mass scaling would let you set a floor for the critical time step that is enforced at each step of the simulation. This will guarantee that the simulation will not run any slower than desired and cannot stall. Thus in both cases, mass scaling offers a unique tool to decrease the required computation time with little change to the simulation’s accuracy. To gain access to this capability for our modeling efforts, mass
scaling has been implemented into the Summit computation solid mechanics solver.

This chapter will continue by providing the theory behind mass scaling in Section 7.1. The section will also provide a description of our implementation of mass scaling into Summit. In section 7.2, a small example of the application of mass scaling is shown.

7.1 Theory

Mass scaling works on a basic principle, but the implementation can vary. The implementations fall into two broad categories: conventional and selective mass scaling. In each, artificial inertia forces are added to the simulations. Conventional mass scaling adds the influence of these forces to all the eigenfrequencies of the dynamics problem, while selective only influences the higher eigenfrequencies \[42\]. By avoiding the lower eigenfrequencies, which correspond to structural deformation, more artificial mass can be added through selective mass scaling than conventional mass scaling before the accuracy of the simulation is affected. However, selective mass scaling does require the use of a non-diagonal mass matrix, which requires extra computations. For simplicity and as a first attempt, the implementation in this study will focus on conventional mass scaling.

To start, the critical time step is based on how long it takes for stress waves to propagate through an element and is computed as

\[ dt_{crit} = t_f \min_{e \in \Omega} \min_{qp \in e} \frac{h_e}{c_{qp}}, \]

where \(t_f\), \(e\), \(qp\), \(h\), and \(c\) are a time factor \((t_f \leq 1)\), the element, the quadrature point, the inscribed radius of the element, and the celerity of the material at the quadrature point, respectively. Thus, it is a quantity based both on the geometry and material parameters. Therefore, to increase the time step to a desired value there are two options: increase the inscribed radius or decrease the celerity. The first options is computationally expensive and difficult to perform because it would require remeshing during the simulation. However,
the second option is relatively simple to perform and computationally cheap, so mass scaling utilizes the alteration of a material’s celerity.

In general, the celerity of a material has the form

\[ c = \frac{\partial p}{\partial \rho} \propto \frac{1}{\sqrt{\rho}}, \]  

(7.1)

where \( p \) and \( \rho \) are pressure and material density, respectively. Clearly, to have a decrease in celerity an increase in \( \rho \) (mass) is required. Without knowledge of the exact form of celerity for a given material, the required density for a desired time step can still be calculated by starting with the relation

\[ \frac{dt_{desired}}{dt_{current}} = \frac{h}{c_{desired}} = \frac{c_{current}}{c_{desired}} = \sqrt{\frac{\rho_{desired}}{\rho_{current}}}. \]  

(7.2)

Equation 7.2 then can be rearranged such that the desired density is expressed as

\[ \rho_{desired} = \left( \frac{dt_{desired}}{dt_{current}} \right)^2 \rho_{current}. \]  

(7.3)

Thus, the density of the critical element is increased by a factor that is the square of the factor of increase in the critical time step when mass scaling is applied. Based on this, conventional mass scaling is a tool that should be applied judiciously and is not appropriate in all situations. The elements undergoing scaling should not represent a significant portion of the overall volume and ideally would not be in critical locations in the mesh as they can act like rigid bodies. Furthermore, artificially increasing the mass modifies the energies in the simulations distorting the overall outcome of the simulations. These distortions become more pronounced at higher rates and with the addition of more mass. In general, this limits the use of conventional mass scaling to quasi-static or low rate simulations. As for an allowable increase in step size, this tool provides a trade-off between the accuracy of a simulation and computation time, and one should choose the level of distortions that they deem acceptable for the task they have on hand.
7.1.1 Implementation in Summit

To implement conventional mass scaling, additions were made to Summit’s source code in several locations. The major addition was in the implementation of the method *StableTimeStepMassScale* in the Mechanics Region class. This method takes in a user designated time floor for the simulation, and it then determines and sets the required density of the element based on Eq. 7.3. Users can set their desired time threshold in an application driver by using the methods *StepMassScale* & *GetTimeIntegratorStableTimeStepMassScale* from the Explicit Newmark Integrator class instead of their non-mass scaling counterparts.

In addition, a new parametric material, *ElasticMassScale*, was defined within the materials library and assigned an identification value at the top level of the material code. The material is an isotropic linearly elastic and has the ability to use a parametrically changing material density.

7.2 Mass Scaling Example: The Propagation of a Stress Wave

As an illustration of mass scaling’s potential, let us examine the simulation shown in Figures (7-3)-(7-8). It was a simulation of a stress wave propagating through a 2D mesh from the right to the left. The mesh was intentionally generated to have a few sliver elements located near its center, which brings down the critical time step of the simulation compared to that of a simulation with an uniform mesh. The nominal critical time step of the simulation with the sliver elements was $1.41 \times 10^{-7}$ seconds. In comparison, a simulation using an uniform mesh would have a critical time step of $1.67 \times 10^{-6}$ seconds. The simulation used a linear elastic material model with Young’s modulus(E), Poisson’s ration($\nu$), and density of 10 GPa, 0.25, and 1000 $\frac{kg}{m^3}$, respectively. Finally, the right side of the mesh was being compressed towards the left at a strain rate of 0.1 $s^{-1}$ while the left side was fixed in place.

This simulation was ran once with and without mass scaling applied. For the mass scaling
run, a critical time step floor of $7.50 \times 10^{-7}$ s was set, which resulted in a reduction of the computation time by approximately a factor of 5.32. This choice for the critical time step led to the mass distribution seen in Figure 7-2. The few very poorly conditioned sliver elements have their density increased to $2.835 \times 10^4 \frac{kg}{m^3}$ while the element that transition back towards an uniform mesh also exhibited a slight increase to their density.

Figure 7-2: The increase in the density after mass scaling is applied to a dynamic simulation. A large increase in density is present in the lowest quality sliver elements along with a smaller increase in the density in other low quality elements surrounding it. (Left) Full mesh for the simulation. (Right) Cutout around the intentionally placed sliver element.

Comparing the simulation results, the 2D stress profiles are qualitatively close overall, but there are still discrepancies in the results. Upon closer examination, the largest discrepancies are located in the region surrounding the sliver elements after the stress wave had passed. This observation can be explained by the fact that mass scaled elements act partially as rigid bodies. A stress wave that interacts with these rigid elements would be impeded, which can be seen occuring in this simulation in Figures 7-5 & 7-6. This impedance leads to localized discrepancies around the sliver elements. However, after a short distance from the impedance the wave front recovered resulting in similar stresses in the regions away from the sliver elements, see Figure 7-7.

In conclusion, this is a simple example, but it illustrates the benefits that mass scaling can provide. Only small discrepancies in the final stresses were present between the mass scaled and non-mass scaled simulation away from the sliver elements. There is a slightly
larger variation between the two simulations in the region near sliver element. However, these discrepancies were paired with reduction in the computation time, in this case a factor of approximately 5.32. If the sliver elements do not constitute a large portion of the mesh and the small variations from the nominal results are acceptable, mass scaling provides a useful tool to increase the speed of dynamic simulations.

Figure 7-3: Comparison of Stress Wave Propagation at $8.0 \times 10^{-5}$s. (Left) Simulation with mass scaling applied. (Right) Non-mass scaled simulation. The stress wave approaching the sliver elements.

Figure 7-4: Comparison of Stress Wave Propagation at $1.3 \times 10^{-4}$s. (Left) Simulation with mass scaling applied. (Right) Non-mass scaled simulation. The stress wave passing through the sliver elements.
Figure 7-5: Comparison of Stress Wave Propagation at $1.5 \times 10^{-4}$s. (Left) Simulation with mass scaling applied. (Right) Non-mass scaled simulation. The stress wave passed through the sliver elements, and for the mass scaled simulation the wave is impeded by the increase in mass.

Figure 7-6: Comparison of Stress Wave Propagation at $1.8 \times 10^{-4}$s. (Left) Simulation with mass scaling applied. (Right) Non-mass scaled simulation. The stress wave is still moving to the left, and for the mass scaled simulation the wave front is still disrupted.

Figure 7-7: Comparison of Stress Wave Propagation at $2.2 \times 10^{-4}$s. (Left) Simulation with mass scaling applied. (Right) Non-mass scaled simulation. The stress wave is still moving to the left, but now the wave front from the mass scaled simulation has reformed.
Figure 7-8: Comparison of Stress Wave Propagation at $2.8 \times 10^{-4}$s. (Left) Simulation with mass scaling applied. (Right) Non-mass scaled simulation. The stress wave reaches the left side of the mesh, and the results of the two simulations are close even though the mass scaled simulation is 5.32 times faster than the non-mass scaled simulation.
Chapter 8

Conclusions

While not all the goals of this study have been achieved, significant progress towards their fulfillment have been made. Two of the four steps in the simulation-based approach to describe the constitutive response of cranial bone in mammals have been completed. First, the microstructure specimen MP14002-11 has been explicitly characterized through the generation of biofidelic meshes.

Second, the Ogden hyperfoam model was determined to be an excellent candidate for describing the constituent material response of Göttingen minipig cranial bone. A detailed finite element model using the hyperfoam model for the constituent was able to capture both the stress-strain response and strain localization observed experimentally. Currently, this constitutive model requires further calibration to fully capture the experimental response at higher strain levels. Once the calibration is completed, the full-resolution microstructure models can begin being validated against the remaining experimental data provided by ARL.

The fourth step to create a homogenized macroscopic model for cranial bone has also progressed. The results presented in this study suggest that a homogenized macroscopic finite element model based on a linear elastic material model with a varying elastic modulus along the depth is insufficient to model cranial bone. Thus, a more complex homogenized model needs to be examined to capture the mechanical response and strain localization.
observed experimentally in cranial bone.

8.1 Future Work

There are several areas of this research that would be beneficial to continue. Three specific areas are determining a representative volume element (RVE) size for cranial bone, modeling intermediate and high strain rate test, and finally, the creation of a homogenized macroscopic finite element model for the cranial bone of Göttingen minipigs. These areas of recommended future work are outlined in more detail below.

8.1.1 Comparison of Representative Volume Elements

For a microscopic finite element model of cranial bone, the simulated response is a combination of the both the structure of the mesh and the constitutive model used. However, the parameters for the constitutive model tend to be calibrated to match the response using a specific mesh. The meshes used for calibration can be a subsection of the overall mesh for the purpose of speeding up the calibration process. If these subsections are not representative of the overall structure, the calibration of the constitutive parameters would be off when returning to the full mesh. It is important to ensure that the meshes used in the calibration process are representative of the overall structure that will be simulated.

Specifically in this study, a \( \frac{1}{64} \) th crop of the full mesh was used. A thorough verification of a representative volume element (RVE) size of cranial bone should be completed. The verification should examine both the size of the subsection and position of the subsection in the overall structure to determine the appropriate RVE to use for the simulations.

8.1.2 Intermediate and High Strain Rate Modeling

A long term goal of this research is to model cranial bone at various strain rates, which range from quasi-static to blast loading. The work completed thus far has been for the quasi-static regime, and the chosen material model has no rate dependency. A step towards
creating a better microscopic finite element model would be the addition of viscous effects into the Ogden hyperfoam model.

8.1.3 Macroscopic modeling for large scale simulations

The creation of a comprehensive macroscopic finite element model for Göttingen minipig cranial bone is another crucial step moving forward. To capture both the experimental stress-strain response and the strain localization, a more complex homogenized model than a purely linear elastic homogenized model will need to be developed. We believe that the Ogden hyperfoam model could be a good starting point for this model. A model of the form expressed in Equation 8.1.3 may be sufficient to model the cranial bone. Additionally, examining $\eta(f_{bv}) = f_{bv}$ would be a good starting place, but a literature review for more comprehensive functions based on bone volume fraction ($f_{bv}$) should be completed.

$$S_{f, J}^{\text{Bone}} = \eta(f_{bv})S_{f, J}^{\text{Ogden}}$$ (8.1)
Appendix A

Ogden Hyperfoam Material Derivations

This appendix provides a derivation for the stress tensor, tangent moduli, and celerity of the Ogden hyperfoam model from its strain energy density function. To be consistent with the Summit finite element framework, the stress tensor is the first Piola-Kirchhoff stress tensor and the tangent is the Lagrangian tangent. Much of this derivation was assisted by previous work by Ogden [44] [45] and Holzapfel [46]. In this derivation, the lower-case subscripts \((i)\) represent the spatial configuration and upper-case subscripts \((I)\) represent the reference configuration.

A.1 Introduction

To start, the strain energy density function for Ogden hyperfoam is expressed as

\[
\psi = \sum_{i=1}^{N} \frac{2\mu_i}{\alpha_i^2} \left[ \lambda_1^{\alpha_i} + \lambda_2^{\alpha_i} + \lambda_3^{\alpha_i} - 3 + \frac{1}{\beta_i} \left( J^{-\alpha_i \beta_i} - 1 \right) \right],
\]

(A.1)

where
\[ \beta_i = \frac{\nu_i}{1 - 2\nu_i} \quad (A.2) \]
\[ J = \lambda_1 \lambda_2 \lambda_3 = det(F) \quad (A.3) \]
\[ C = \sum_{a=1}^{3} \lambda_a^2 \hat{N}_a \otimes \hat{N}_a \quad (A.4) \]

Each term in the series has three variables \( \mu_i, \nu_i, \) and \( \alpha_i \). They represent the shear modulus, Poisson’s ratio, and a dimensionless parameter for each term in the series. \( \lambda_a \) and \( \hat{N}_a \) represent the principal stretches and principal stretch directions, respectively.

Additionally, from the input parameters the initial shear modulus and bulk modulus for the overall material response are given as
\[ \mu_0 = \sum_{i=1}^{N} \mu_i \quad (A.5) \]
\[ K_0 = \sum_{i=1}^{N} 2\mu_i \left( \frac{1}{3} + \beta_i \right). \quad (A.6) \]

### A.2 First Piola-Kirchhoff Stress Tensor

In terms of the strain energy function \( \psi \), the second Piola-Kirchhoff stress may be written as
\[ S = 2 \frac{\partial \psi}{\partial C} \quad \text{or} \quad S_{IJ} = 2 \frac{\partial \psi}{\partial C_{IJ}}. \quad (A.7) \]

The strain energy function can be decomposed into two terms: one dealing with the stretches and one dealing with the Jacobian \( \psi_\lambda \) and \( \psi_{\text{jac}} \) with \( \psi = \psi_\lambda + \psi_{\text{jac}} \). Based on this, the expression for stress becomes
\[ S_{IJ} = 2 \left[ \frac{\partial \psi_\lambda}{\partial C_{IJ}} + \frac{\partial \psi_{\text{jac}}}{\partial C_{IJ}} \right]. \quad (A.8) \]
Equation A.8 can then be expanded to

\[ S_{IJ} = 2 \sum_{a=1}^{3} \left( \frac{1}{2\lambda_a^2} \frac{\lambda_a^2}{\partial \psi_{\lambda_a} \partial C_{IJ}} \right) + \frac{\partial \psi_{jac}}{\partial J} \frac{\partial J}{\partial C_{IJ}} \]  

(A.9)

where

\[ \psi_{\lambda} = \sum_{i=1}^{N} \sum_{a=1}^{3} \frac{2\mu_i}{\alpha_i^2} \left[ \lambda_a^{\alpha_i} - 1 \right] \]  

(A.10)

\[ \psi_{jac} = \sum_{i=1}^{N} \frac{2\mu_i}{\alpha_i^2 \beta_i} \left[ J^{-\alpha_i \beta_i} - 1 \right]. \]  

(A.11)

The intermediate terms in Equation A.9 are expressed as

\[ \frac{\partial \psi_{\lambda}}{\partial \lambda_a} = \sum_{i=1}^{N} \frac{2\mu_i}{\alpha_i} \lambda_a^{\alpha_i - 1} \]  

(A.12)

\[ \frac{\partial \lambda_a^2}{\partial C_{IJ}} = \hat{e}_I \cdot \frac{\partial \lambda_a^2}{\partial C} \hat{e}_J = \hat{e}_I \cdot (\tilde{N}_a \otimes \tilde{N}_a) \hat{e}_J = (\tilde{N}_a \cdot \hat{e}_J) (\tilde{N}_a \cdot \hat{e}_J) \]  

(A.13)

\[ \frac{\partial \psi_{jac}}{\partial J} = - \sum_{i=1}^{N} \frac{2\mu_i}{\alpha_i} (J^{-\alpha_i \beta_i - 1}) \]  

(A.14)

\[ \frac{\partial J}{\partial C_{IJ}} = \frac{J}{2} C_{IJ}^{-1}. \]  

(A.15)

In Equation A.13, the expression for \( \frac{\partial \lambda_a^2}{\partial C} \) is from Equation 2.125-128 in [46] by Holzapfel.

By substituting Equations A.12, A.13, A.14, & A.15 into Equation A.9, the final form of the second Piola-Kirchhoff stress is expressed as

\[ S_{IJ} = 2 \sum_{i=1}^{N} \frac{\mu_i}{\alpha_i} \left[ \sum_{a=1}^{3} \left( \lambda_a^{\alpha_i - 2} (\tilde{N}_a \cdot \hat{e}_J)(\tilde{N}_a \cdot \hat{e}_J) \right) - C_{IJ}^{-1} J^{-\alpha_i \beta_i} \right]. \]  

(A.16)

For use later in the derivation, we will decompose the stress as follows

\[ S_{IJ} = S_{\lambda_{IJ}} + S_{jac_{IJ}}, \]  

(A.17)
where
\begin{align}
S_{\lambda_{IJ}} &= 2 \sum_{i=1}^{N} \frac{\mu_i}{\alpha_i} \sum_{a=1}^{3} \lambda_a^{\alpha_i-2} (\tilde{N}_a \cdot \hat{e}_I)(\tilde{N}_a \cdot \hat{e}_J) \quad (A.18) \\
S_{jac_{IJ}} &= -2 \sum_{i=1}^{N} \frac{\mu_i}{\alpha_i} C_{IJ}^{-1} J^{-\alpha_i} \beta_i. \quad (A.19)
\end{align}

For use in Summit, the first Piola-Kirchhoff Stress is desired. This would simply be
\[
P_{iJ} = F_{iJ} S_{IJ}. \quad (A.20)
\]

### A.3 Lagrangian Tangent

The next quantity to be derived is the material moduli, which will then be transformed to the Lagrangian tangent for use by Summit. The material tangent can be derived from the strain energy function by

\[
C_{IJKL} = 2 \frac{\partial S_{IJ}}{\partial C_{KL}} = 4 \frac{\partial^2 \psi}{\partial C_{IJ} \partial C_{KL}}. \quad (A.21)
\]

Decomposing the tangent into two parts, as was done with the strain energy function, results in the expression

\[
C_{IJKL} = C_{\lambda IJKL} + C_{jac IJKL}. \quad (A.22)
\]

First, using Equation 6.180 of [46], the tangent corresponding to the principal stretches can be defined as

\[
C_{\lambda IJKL} = \sum_{a,b=1}^{3} \frac{1}{\lambda_a \lambda_b} \frac{\partial S_a}{\partial \lambda_a} (\tilde{N}_a \cdot \hat{e}_I)(\tilde{N}_a \cdot \hat{e}_J)(\tilde{N}_b \cdot \hat{e}_K)(\tilde{N}_b \cdot \hat{e}_L) + \sum_{a,b=1, a \neq b}^{3} \frac{S_b - S_a}{\lambda_b^2 - \lambda_a^2} [(\tilde{N}_a \cdot \hat{e}_I)(\tilde{N}_b \cdot \hat{e}_J)(\tilde{N}_a \cdot \hat{e}_K)(\tilde{N}_b \cdot \hat{e}_L) + (\tilde{N}_a \cdot \hat{e}_I)(\tilde{N}_b \cdot \hat{e}_J)(\tilde{N}_b \cdot \hat{e}_K)(\tilde{N}_a \cdot \hat{e}_L)]. \quad (A.23)
\]

This general form (Equation A.23) is specialized to the Ogden hyperfoam model, by defin-
ing the following terms.

\[
S_a = \sum_{i=1}^{N} \frac{2\mu_i}{\alpha_i} \lambda^{\alpha_i - 2}
\]  
(A.24)

\[
\frac{\partial S_a}{\partial \lambda_b} = \sum_{i=1}^{N} \frac{2\mu_i}{\alpha_i} (\alpha_i - 2) \lambda^{\alpha_i - 3} \delta_{ab}
\]  
(A.25)

Additionally, if \( \lambda_a = \lambda_b \), the use of L'Hôpital's rule is required to avoid indeterminacy in the second term in Equation A.23. The second term can then be expressed as

\[
\lim_{\lambda_b \to \lambda_a} \frac{S_b - S_a}{\lambda_b^2 - \lambda_a^2} = \frac{\partial S_b}{\partial \lambda_b} - \frac{\partial S_a}{\partial \lambda_b}
\]  
(A.26)

which, when specialized to the Ogden hyperfoam becomes

\[
\lim_{\lambda_b \to \lambda_a} \frac{S_b - S_a}{\lambda_b^2 - \lambda_a^2} = \sum_{i=1}^{N} \frac{\mu_i}{\alpha_i} (\alpha_i - 2) \lambda_a^{\alpha_i - 4}
\]  
(A.27)

Next, the tangent corresponding to the Jacobian can be expressed as

\[
C_{jaci,JKL} = 2 \frac{\partial S_{jaci}}{\partial C_{KL}}
\]  
(A.28)

Based on Equation A.19, \( \frac{\partial S_{jaci}}{\partial C_{KL}} \) may be expressed as

\[
\frac{\partial S_{jaci}}{\partial C_{KL}} = -2 \sum_{i=1}^{N} \frac{\mu_i}{\alpha_i} \left[ \frac{\partial C_{ii}}{\partial C_{KL}} J^{-\alpha_i \beta_i} + C_{iJ}^{-1} \frac{\partial J^{-\alpha_i \beta_i}}{\partial J} \frac{\partial J}{\partial C_{KL}} \right].
\]  
(A.29)

The intermediate terms in Equation A.29 are expressed by

\[
\frac{\partial C_{ii}^{-1}}{\partial C_{KL}} = -\frac{1}{2} \left[ C_{ik}^{-1} C_{ij}^{-1} + C_{ij}^{-1} C_{ik}^{-1} \right]
\]  
(A.30)

\[
\frac{\partial J}{\partial C_{KL}} = \frac{J}{2} C_{KL}^{-1}
\]  
(A.31)
Combining Equations A.28, A.29, A.30, & A.31 results in the expression

\[ C_{jacIJKL} = 2 \sum_{i=1}^{N} \mu_{i} \left( \frac{1}{\alpha_{i}} J^{\alpha_{i}\beta_{i}} \left[ C_{IKL}^{-1} C_{LJ}^{-1} + C_{ILJ}^{-1} C_{JKL}^{-1} \right] - C_{IJL}^{-1} C_{KJKL}^{-1} \beta_{i} J^{\alpha_{i}\beta_{i}} \right) \]  \hspace{1cm} (A.32)

which is the final form for the component of the material tangent dealing with the Jacobian.

This completes the derivation of the material tangent. For Summit, the Lagrangian tangent is required, and it can be expressed in terms of the material tangent as

\[ C_{ijkl} = \frac{\partial P_{ij}}{\partial F_{kL}} = \delta_{ik} S_{jL} + C_{IJKL} F_{iL} F_{kK}. \]  \hspace{1cm} (A.33)

**A.4 Material Celerity**

The final quantity to be derived for the Ogden hyperfoam model is the material’s celerity. The celerity is required to compute the stable time step for an explicit simulation, which makes it a crucial quantity used by Summit. This derivation starts by first defining pressure as

\[ p = \frac{1}{3} tr\sigma = \frac{1}{3} tr(J^{-1}F SF^T). \]  \hspace{1cm} (A.34)

Next, the square of celerity is defined as the derivative of the pressure with respect to the density of the material in Equation A.35.

\[ c^2 = \frac{\partial p}{\partial \rho} = \frac{\partial p}{\partial J} \frac{\partial J}{\partial \rho} \]  \hspace{1cm} (A.35)

Plugging in the expression for pressure into Equation A.35, results in

\[ c^2 = \frac{1}{3} tr(J^{-1}F SF^T) \frac{\partial J}{\partial \rho} = \frac{1}{3} tr(J^{-1}F(S + S_{jac})F^T) \frac{\partial J}{\partial \rho}. \]  \hspace{1cm} (A.36)

The intermediate terms in Equation A.36 are defined by

\[ \frac{1}{3} tr(J^{-1}F S_{a} F^T) = -\frac{2}{3J^2} \sum_{i=1}^{N} \sum_{a=1}^{3} \mu_i \lambda_{ai} \left[ \frac{1}{\alpha_i} + 1 \right] \]  \hspace{1cm} (A.37)
\[
\frac{\partial}{\partial J} \text{tr}(J^{-1} FS_{jac} F^T) = -2 \sum_{i=1}^{N} \frac{\mu_i}{\alpha_i} (-\alpha_i \beta_i - 1) J^{-\alpha_i \beta_i - 2}
\]
(A.38)

\[
\frac{\partial J}{\partial \rho} = -\rho_0 \rho^{-2} = -J^2 \rho_0^{-1},
\]
(A.39)

where the Jacobian is defined as \( J = \frac{\partial \mathbf{\xi}}{\partial \rho} \). With these, Equation A.36 becomes

\[
c^2 = -2 \rho_0^{-1} \sum_{i=1}^{N} \mu_i \left[ \frac{1}{\alpha_i} (\alpha_i \beta_i + 1) J^{-\alpha_i \beta_i} - \frac{1}{3} \sum_{a=1}^{3} \lambda_a^{\alpha_i} (\frac{1}{\alpha_i} + 1) \right].
\]
(A.40)

Finally, the celerity of the Ogden hyperfoam model may be expressed as

\[
c = \sqrt{-2 \rho_0^{-1} \sum_{i=1}^{N} \mu_i \left[ \frac{1}{\alpha_i} (\alpha_i \beta_i + 1) J^{-\alpha_i \beta_i} - \frac{1}{3} \sum_{a=1}^{3} \lambda_a^{\alpha_i} (\frac{1}{\alpha_i} + 1) \right]}
\]
(A.41)

by taking the square root of Equation A.40.
Appendix B

Material Consistency Test

Implementation of a constitutive model into a finite element package can be a complex task, and verification of the implementation should be completed to check for mistakes. For a variational constitutive model, there is a simple set of tests that can be performed for verification. The first test is to check for consistency between the implementation the stress and the strain energy function, and the second test is to check for consistency between the implementation of the tangent and the stress. In Summit, the consistency tests are specifically for the first Piola-Kirchhoff stress and the Lagrangian tangent. Both the tests are based on the finite difference method and are outlined in their respective sections.

B.1 First Piola-Kirchhoff Stress Consistency Test

To test for consistency between the strain energy equation and the stress tensor, let us first look at the definition of the first Piola-Kirchhoff stress for a variational model. The first Piola-Kirchhoff stress is defined as

\[ P(F) = \frac{\partial \psi(F)}{\partial F}, \quad \text{(B.1)} \]

or in index notation as

\[ P_{ij}(F') = \frac{\partial \psi(F)}{\partial F_{ij}}. \quad \text{(B.2)} \]

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If one applies the second order central difference method to the first Piola-Kirchhoff stress, the equation would become

\[
P_{ij}(F) \approx P_{ij}^h(F) = \frac{\psi(F + h e_i \otimes e_j) - \psi(F - h e_i \otimes e_j)}{2h} + O(h^2), \tag{B.3}
\]

where \(h\) is a small perturbation (i.e. an order of \(1 \times 10^{-6}\) times smaller than the dominant term in the deformation gradient) of \(F\). \(P(F)\) will be referred to as the analytical stress tensor, and \(P^h(F)\) will be referred to as the numerical stress tensor. The analytical stress tensor represents your implementation of the variational constitutive model. The numerical stress tensor will be used for comparison because it is computed from only \(\psi\), which is the starting point of the analytical derivation.

The actual consistency test for stress is to check that the condition

\[
|P_{ij} - P_{ij}^h| \leq O(h^2) \tag{B.4}
\]

is met. The test should be run for a variety of deformation gradients and constitutive parameters to ensure that the implementation of the variational constitutive model is robust.

### B.2 Lagrangian Tangent Consistency Test

Similar to the stress tensor, a consistency test can also be performed for the Lagrangian tangent. To start, the Lagrangian tangent can be expressed as

\[
\mathbb{C}(F) = \frac{\partial P(F)}{\partial F}, \tag{B.5}
\]

or in index notation

\[
\mathbb{C}_{ijkl}(F) = \frac{\partial P_{ij}(F)}{\partial F_{kl}}. \tag{B.6}
\]

Applying the finite difference method to the expression for the tangent results in

\[
\mathbb{C}_{ijkl}^h(F) = \frac{P_{ij}(F + he_k \otimes e_L) - P_{ij}(F - he_k \otimes e_L)}{2h} + O(h^2). \tag{B.7}
\]
Analogous to the stress consistency test, the consistency test for the Lagrangian tangent is to ensure that the condition

\[ |C_{ijkl} - C^h_{ijkl} | \leq \mathcal{O}(h^2) \]  \hspace{1cm} (B.8)

is met for a variety of deformation gradients and constitutive parameters.
Bibliography


[31] ANSYS Academic Research, Release 15.0, ANSYS, Inc.


