COMPUTATIONAL DESIGN AND ANALYSIS OF MULTI-SCALE POLYMER MACHINES

BY

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THESIS
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ABSTRACT

This thesis discusses the computational analysis of multi-scale polymer systems for a variety of applications. Two geometries are analyzed, polymer sheets that fold into complex shapes due to a gradient in cross-linking throughout its volume, and a dome structure that experiences limit point buckling during inversion.

The first chapter of this work discusses an analysis of the self-assembly of thin, programmable Polydimethylsiloxane (PDMS)/SU-8 sheets, which fold due to complex swelling ratio gradients throughout their volume. These could be used as a fabrication technique for small polymer devices or as a means of actuation in a polymer machine. An analytical elasticity model and a computational model in ABAQUS/Standard are used to predict the direction of folding for different sheet specimens. The model is also used to analyze specimens with more complex time varying deformations.

Next a dome structure is investigated for its potential use as the scaffold of a biomechanical machine powered by cells. The machines are millimeter sized and are actuated by groups of cells cultured on the machine. These biological machines have important potential applications for drug delivery or chemical sensing. Finite element analysis is used to study these domes so that an optimal biological machine can be designed.
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CHAPTER 1: MECHANISTIC MODEL OF PDMS/SU-8 SHEET SELF ASSEMBLY

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1.1. Introduction

Complex deformation of materials can be induced or controlled by differential straining of patterned structures at a variety of sizes all the way down to the nanoscale. Common driving forces for this deformation include capillary action \cite{1-3}, epitaxial mismatch strain \cite{4-6}, and differences in solvent swelling \cite{7-14}. One special case of these phenomena is the folding of thin plates or beams due to a gradient in strain. This phenomenon can be used as a fabrication technique at small scales, when common deformation techniques are impermissibly time consuming and expensive. Chun et al. \cite{4} recently used epitaxial mismatch strain to quickly and reliably create thousands of semiconductor micro-rings for use in electronics. Gradients in normal strain have also been used to fabricate microfluidic devices \cite{7-8}, microelectronic systems \cite{2-4}, and capsules capable of catching and releasing cells or drugs \cite{9-11}.

In order to realize the potential of this fabrication technique, a predictive computational model is essential. Such a model could be used to design simple substrates that fold into complex

a: Performed experiments related to the computation, including taking experimental images.
b: Independently made Figures 1.1.2b,1.2c, and the non-computational sheet renderings in Figure 1.3a.
c: Helped develop some of the analytical solution described in 1.3.2.
d: Main research advisor
The deformation of thin sheets due to gradients in strain has been studied with a variety of analytical and computational models. Past work has focused on using an analytical energy model \([1,2,5,14,15,16]\) and a computational model \([4,5,10,12,14]\) to determine the direction of folding for different bilayer sheet shapes with varying levels of normal strain mismatch. Recently Stoychev et al. \([14]\) modeled the progression of swelling ratio through the volume of polymer sheets with a heat transfer model. Because heat transfer is governed by similar differential equations, they could use this model to understand how these sheets deform. Although past work has been done to study deformation modes in thin polymer systems, further work is necessary to understand how more complex gradients in swelling ratio throughout a specimen’s volume affect overall deformation modes.

Motala \([17]\), and Yuan \([18]\) developed an experimental setup used to construct polymer specimens with complex swelling ratio gradients through their volume. By selectively cross-linking specimens, polymer systems with complex deformation modes were designed. In this work, the previous fabrication procedure and a unique deformation mode are reviewed. A mechanistic model used to analyze the system is described in detail, and the model is used to analyze systems that actuate quickly due to a buildup of residual stress.

1.2. Observations and Mechanisms

1.2.1 Experimental Specimen Fabrication

Motala \([17]\), and Yuan \([18]\) developed an experimental method based on the concept of differential swelling to control deformation of polymer sheets. To fabricate the programmable sheets that can fold in various modes, a mixture of Polydimethylsiloxane (PDMS) and SU-8-
photoresist was used. The mixture was spin coated on a glass slide and then heated to allow the PDMS to cross-link. A photo mask was used to selectively expose the SU-8 in the PDMS to UV light, creating spatial distribution of different cross-link density both within the plane, and through the thickness of the sheet. To determine how the cross-linking profile varies through the thickness of the sheet specimens, the final PDMS samples were exposed to Rhodamine 6G, a fluorescent dye that is most absorbed by the region unexposed to UV light. As a result, under fluorescence excitation, the SU-8 cross-linked section is darker than the rest of the sheet. A fluorescent microscope was used to image the material’s cross-section and determine the cross-link density distribution. The resulting profile was used to assign the spatial distribution of material properties used in the analysis of the sheet’s mechanical responses. The fluorescent image is shown in Figure 1.1a below. The degree of darkness in Figure 1.1.a corresponds directly to the local cross-linking density. This profile creates three general material sections: the heavily SU-8 cross-linked (XL) section, the non-SU-8 cross-linked (NXL) section, and the partially SU-8 cross-linked (PXL) section, which are labeled in Figure 1.1a.
The elastic modulus of the material was measured across the entire top and bottom surface of a sheet with atomic force microscopy (AFM) before immersing it in toluene. Elasticity values were averaged for each section of the sheet. Swelling ratio, $\lambda$, was measured for a sheet fully exposed to light, XL material, and a sheet unexposed to light, NXL material, as described by

$$\lambda = \frac{l_f}{l_i}$$  \hspace{1cm} (1.1)

where $l_f$ is the final length a swelled sample and $l_i$ is the initial length. The PDMS literature value of 0.499 was used for the Poisson’s Ratio of each material section [19]. From past work it is also known that highly cross-linked materials have higher elastic moduli, lower swelling ratio [20], and absorb solvent more slowly [21]. These results are shown in Table 1.1.
Table 1.1: Measured Elastic Properties. Yuan and Daly measured elasticity and swelling ratio

<table>
<thead>
<tr>
<th>Sheet Section</th>
<th>Elasticity (MPa)</th>
<th>Poisson’s Ratio</th>
<th>Swelling Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>XL</td>
<td>15.44 (High)</td>
<td>0.499</td>
<td>1.171 (Low)</td>
</tr>
<tr>
<td>NXL</td>
<td>2.32 (Low)</td>
<td>0.499</td>
<td>1.53 (High)</td>
</tr>
<tr>
<td>PXL</td>
<td>11.63 (Medium)</td>
<td>0.499</td>
<td>[-] (Medium)</td>
</tr>
</tbody>
</table>

1.2.2. Idealized Model and Deformation Mechanisms

It is assumed in this work that each section of different cross-link density is a linear elastic isotropic material with the mechanical properties given in Table 1.1, and the full sheet is made of these separate materials joined together. Figure 1.1b shows a depiction of the cross-linking profile through the sheet cross-section and an idealized model of XL, PXL, and NXL sections.

An analysis of Figure 1.1a in MATLAB gave the cross sectional dimensions shown in Figure 1.1b. When the spacing of the cross-linked sections is low, the PXL sections on the bottom layer overlap, forming a uniform partially cross-linked layer. These materials create cross-linked bilayers (XLB) and non-cross-linked bilayers (NXLB) along the entire sheet. The bilayers are labeled in Figure 1.2a. Figure 1.2b shows a depiction of the final sheet configuration.
When this composite sheet is immersed in toluene, different sections swell by a different amount. The NXL section has the highest swelling ratio, the PXL an intermediate swelling ratio, and XL the lowest swelling ratio. The mismatched strain created due to differential swelling between the layers of the system allows the sheet to fold in different directions. Only two folding directions...
were observed experimentally and computationally, folding around the axis parallel to the XL lines with the PXL material facing inward, and folding around the axis perpendicular to the XL lines with the PXL material facing outward. These deformation modes are shown in Figure 1.2c and will henceforth be referred to as Folding Mode 1 and Folding Mode 2 respectively.

Under certain conditions the specimens deformed into Folding Mode 1, unfolded, and then deformed into Folding Mode 2. This work seeks to use mechanistic models to understand the double folding phenomena.

1.3. Uniform Swelling Methods

Both numerical and analytical methods are employed in the study of the deformation of the selectively cross-linked sheet upon differential swelling. The numerical analysis is carried out using the finite element method. The analytical model uses a composite theory with effective elastic and swelling properties. Two swelling processes are considered: the idealized case of uniform swelling throughout the entire sheet, and the transient process as swelling propagates from the surfaces to the interior of the sheet.

We first consider the case when the swelling occurs uniformly in each of the components of XL, PXL, and NXL materials. Using a mechanistic model, a state diagram was found describing folding direction from values of elasticity and swelling ratio. These results were used to analyze the change in preferred folding direction during the double folding mode. A finite element model and a corresponding analytical model were developed.
Swelling of each material can be modeled as a predefined swelling strain. A common first order approximation is to assume the swelling strain is a linear function of solvent concentration. This assumption gives

\[ \varepsilon_0 = \frac{C}{C_s} \varepsilon_{0s} \]  

(1.2)

where \( \varepsilon_0 \) is the swelling strain, \( C_s \) is the concentration of solvent at full saturation, and \( \varepsilon_{0s} \) is the swelling strain saturation. An equivalent thermal expansion model can then be used to study swelling, an assumption often used in past work [12,14,22].

### 1.3.1. Finite Element Model

A finite element model in ABAQUS/Standard was used to study the folding modes for our PDMS sheets. A fourth of the 32mm by 32mm by 120\( \mu \)m sheet was modeled, and two axes of symmetry were used. The sheet had 51,200 multilayered shell elements with 4 nodes per element, and 14 integration points through the shell thickness. Integration points through the thickness of the shell element allow the elastic properties of the two materials in each bilayer to be defined. As described by Hu et al. [23], Song et at. [24], and Naceur et al. [25], shell elements offer accuracy and computational efficiency for mechanical problems involving the folding of thin sheets due to a mismatch in normal strain. For all analyses a static algorithm that solves for non-linear deformation with Newton-Raphson iterations was used. Further details on the algorithm have been documented by ABAQUS [26]. The model was validated with a mesh convergence study and a comparison between shell and brick elements for a small sheet. The results show that further mesh refinement did not affect folding direction and that shell and brick elements produced relatively similar results. The comparison between shell and brick elements is described in detail in Section 1.5.3.
In the uniform swelling analysis, a parametric study was carried out by systematically changing the swelling strain and elasticity of the PXL and XL materials. The relationship between material properties, caused by the different levels of cross-linking in each material, as described in Table 1.1, was upheld for all simulations. While keeping the elasticity of the materials constant during each individual analysis, the swelling strain was linearly increased to its final value so that the preferred folding direction is constant throughout the analysis.

1.3.2. Analytical Model

An analytical model was developed to complement the numerical study. The analysis allows for calculation of total strain energy in the system and the preferred folding direction is the deformation mode with lower overall strain energy. To calculate the strain energy of each folding mode, linear elastic theory was used and the top half of the sheet was modeled as a composite made of the NXL material reinforced with the XL material. Hyer [15] and Shokrieh et al. [16] have performed similar analyses to study the shape of composite laminates experiencing a temperature change. For this paper, a derivation by Nishidate et al. was followed who found the stress and strain in a bilayer beam with a mismatch in thermal strain under generalized plane strain [27].

Modeling the top layer of the sheet as a composite laminate allows for a prediction of the effective Young’s modulus and coefficient of thermal expansion for a sheet parallel and transverse to the lines of cross-linked materials. As described by Schapery [28] the rule of mixtures describes the Young’s moduli in each direction, and the strain energy in the composite
layer can be used to derive the effective swelling strain in each direction. The elastic moduli and coefficients of thermal expansion are given by

\[ E_p = V_{XL} E_{XL} + (1 - V_{XL}) E_{NXL}, \]  
\[ E_t = \left( \frac{V_{XL}}{E_{XL}} + \frac{(1-V_{XL})}{E_{NXL}} \right)^{-1}, \]  
\[ \varepsilon_{0p} = \frac{E_{XL} \varepsilon_{0XL} V_{XL} + E_{NXL} \varepsilon_{0NXL}(1-V_{XL})}{E_{XL} V_{XL} + E_{NXL}(1-V_{XL})}, \]

and

\[ \varepsilon_{0t} = \varepsilon_{0XL} + (\varepsilon_{0XL} - \varepsilon_{0p}) v - (\varepsilon_{0XL} - \varepsilon_{0NXL}) (1 + (1 - V_{XL})) \frac{V_{XL} - v}{V_{XL} - (1-V_{XL})} \]

where \( E_p \) is the effective composite elastic modulus parallel to the XL lines, \( E_t \) is the effective composite elastic modulus perpendicular to the XL lines, \( V_{XL} \) is the volume fraction of the XL material, \( E_{XL} \) is the modulus of the XL material, \( E_{NXL} \) is the elasticity of the NXL material, \( v \) is Poisson’s ratio of each material, \( \varepsilon_{0p} \) is the effective swelling strain parallel to the lines of XL material, \( \varepsilon_{0t} \) is the transverse swelling strain, \( \varepsilon_{0XL} \) is the predefined swelling strain in the XL material, and \( \varepsilon_{0NXL} \) is the predefined swelling strain in the NXL material. Given Equations 1.3-1.6 the top half of the sheet was modeled as a homogenized anisotropic material. With this assumption, strain energy was found in a bilayer sheet with a finite nonzero curvature in one direction and zero curvature in the other direction. The direction of nonzero curvature is perpendicular to the XL lines in Folding Mode 1 and parallel to the XL lines in Folding Mode 2.

According to Nishidate, the strain in the direction with a nonzero curvature, denoted here by \( \varepsilon_c \), at a specific cross-section location is given by

\[ \varepsilon_c = \varepsilon_{01} + \frac{y-y_b}{\rho} \]  

where $\varepsilon_{01}$ is the uniform strain component, $y$ is the height from the bottom of the sheet, $y_b$ is the $y$ location of zero bending strain, and $\rho$ is the radius of curvature of the sheet. The strain in the direction with zero curvature is given by an unknown constant $\varepsilon_c$. From Hooke’s law, the stress in Folding Mode 1 is given by

\[
\sigma_{c1} = \frac{E_t(\varepsilon_c - \varepsilon_{0t} + \varepsilon_{0b} y - \varepsilon_{0t} y)}{(1-\nu^2)},
\]

(1.8)

\[
\sigma_{c01} = \frac{E_p(\varepsilon_{0c} - \varepsilon_{0b} + \varepsilon_c y - \varepsilon_{0t} y)}{(1-\nu^2)},
\]

(1.9)

\[
\sigma_{PXLc1} = \frac{E_{PXL}(\varepsilon_c - \varepsilon_{0PXL} + \varepsilon_{0c} y - \varepsilon_{0PXL} y)}{(1-\nu^2)},
\]

(1.10)

and

\[
\sigma_{PXLc01} = \frac{E_{PXL}(\varepsilon_{0c} - \varepsilon_{0PXL} + \varepsilon_c y - \varepsilon_{0PXL} y)}{(1-\nu^2)},
\]

(1.11)

where $\sigma_{c1}$ is the stress in the direction of nonzero curvature in the top layer of the sheet, $\sigma_{c01}$ is the stress in the direction of zero curvature in the top layer of the sheet, $\sigma_{PXLc1}$ is the stress in the direction of nonzero curvature in the PXL layer of the sheet, and $\sigma_{PXLc01}$ is the stress in the direction of zero curvature in the PXL layer of the sheet. The stress in Folding Mode 2 is given by

\[
\sigma_{c2} = \frac{E_p(\varepsilon_{0c} - \varepsilon_{0b} + \varepsilon_c y - \varepsilon_{0t} y)}{(1-\nu^2)},
\]

(1.12)

\[
\sigma_{c02} = \frac{E_t(\varepsilon_c - \varepsilon_{0t} + \varepsilon_{0b} y - \varepsilon_{0t} y)}{(1-\nu^2)},
\]

(1.13)

\[
\sigma_{PXLc2} = \frac{E_{PXL}(\varepsilon_c - \varepsilon_{0PXL} + \varepsilon_{0c} y - \varepsilon_{0PXL} y)}{(1-\nu^2)},
\]

(1.14)

and

\[
\sigma_{PXLc02} = \frac{E_{PXL}(\varepsilon_{0c} - \varepsilon_{0PXL} + \varepsilon_{0c} y - \varepsilon_{0PXL} y)}{(1-\nu^2)}.
\]

(1.15)
where $\sigma_{c2}$ is the stress in the direction of nonzero curvature in the top layer of the sheet, $\sigma_{c02}$ is the stress in the direction of zero curvature in the top layer of the sheet, $\sigma_{PXLc2}$ is the stress in the direction of nonzero curvature in the PXL layer of the sheet, $\sigma_{PXLc02}$ is the stress in the direction of zero curvature in the PXL layer of the sheet, and $E_{PXL}$ is the elastic modulus of the PXL material. Equilibrium equations as described by Nishidate et al. [27] are given by

$$
\int_{y=0}^{h} \sigma_{PXLc01} dy + \int_{y=h}^{2h} \sigma_{c01} dy = 0, 
\tag{1.16}
$$

$$
\int_{y=0}^{h} \sigma_{PXLc1} (y - y_b) dy + \int_{y=h}^{2h} \sigma_{c1} (y - y_b) dy = 0,
\tag{1.17}
$$

$$
\int_{y=0}^{h} \frac{E_{PXL} (y - y_b)}{\rho (1 - v^2)} dy + \int_{y=h}^{2h} \frac{E_{f} (y - y_b)}{\rho (1 - v^2)} dy = 0,
\tag{1.18}
$$

and

$$
\int_{y=0}^{h} \frac{E_{PXL} (\varepsilon_{01} + \varepsilon_{c01} (1 + v) \varepsilon_{0PXL})}{\rho (1 - v^2)} dy + \int_{y=h}^{2h} \frac{E_{f} (\varepsilon_{01} + \varepsilon_{c01} (1 + v) \varepsilon_{0PXL})}{\rho (1 - v^2)} dy = 0,
\tag{1.19}
$$
in Folding Mode 1, and

$$
\int_{y=0}^{h} \sigma_{PXLc02} dy + \int_{y=h}^{2h} \sigma_{c02} dy = 0, 
\tag{1.20}
$$

$$
\int_{y=0}^{h} \sigma_{PXLc2} (y - y_b) dy + \int_{y=h}^{2h} \sigma_{c2} (y - y_b) dy = 0,
\tag{1.21}
$$

$$
\int_{y=0}^{h} \frac{E_{PXL} (y - y_b)}{\rho (1 - v^2)} dy + \int_{y=h}^{2h} \frac{E_{f} (y - y_b)}{\rho (1 - v^2)} dy = 0,
\tag{1.22}
$$

and

$$
\int_{y=0}^{h} \frac{E_{PXL} (\varepsilon_{01} + \varepsilon_{c01} (1 + v) \varepsilon_{0PXL})}{\rho (1 - v^2)} dy + \int_{y=h}^{2h} \frac{E_{f} (\varepsilon_{01} + \varepsilon_{c01} (1 + v) \varepsilon_{0PXL})}{\rho (1 - v^2)} dy = 0,
\tag{1.23}
$$
in Folding Mode 2. Equations 1.16-1.23 can be solved for $\varepsilon_{01}$, $y_b$, $\rho$, and $\varepsilon_{c0}$ in each folding direction. The resulting radius of curvature of Folding Mode 1, $\rho_1$, and Folding Mode 2, $\rho_2$ are given by

$$
\rho_1 = \frac{h (1 + \frac{1}{n_f} + n_t)}{12 \left( \varepsilon_{0t} - \varepsilon_{0PXL} + N (\varepsilon_{op} - \varepsilon_{0PXL}) \right)},
\tag{1.24}
$$
\[ \rho_2 = \frac{h(14 + \frac{1}{n_p} + n_p)}{12 (\varepsilon_{op} - \varepsilon_{p,XL} + \nu(\varepsilon_{ot} - \varepsilon_{o,XL}))} \]  \hspace{1cm} (1.25) 

where \( n_t = E_t / E_{p,XL} \), \( n_p = E_p / E_{p,XL} \), and \( h \) is the height of each layer of the sheet. It is known from these equations that the amount of bending is a function of the difference in swelling strain between the top and bottom layers of the sheet. Using these results, the strain energy, \( U \), for both folding modes is given by

\[ U = \frac{1}{2} \int \sigma_{ij} (\varepsilon_{ij} - \varepsilon_{0,ij}) \, dv \]  \hspace{1cm} (1.26)

where \( \sigma \) and \( \varepsilon \) are the classical stress and strain tensors, and \( \varepsilon_0 \) is the predefined swelling strain tensor. In using an effective swelling strain for the parallel and transverse directions of the sheet, the strain energy caused by the mismatch between the XL and NXL material is ignored. The model assumes that this stress does not cause bending in either direction and is relatively equivalent in both folding modes, so the strain energy of both modes can still be compared. This was validated numerically by analyzing a sheet with only the NXL and XL material without the PXL material below it. It was found that this sheet only deforms in small local regions and does not cause global bending in any direction. Similar assumptions have also been used in past work studying fiber reinforced metal composites [15,16]. The strain energy can be non-dimensionalized by dividing the energy by \( V E_{p,XL} \varepsilon_{0,XL} \) where \( V \) is the volume of the sheet. The resulting equation for the non-dimensional strain energy \( U^*_1 \), of Folding Mode 1 is given by

\[ U^*_1 = \alpha_1 \varepsilon_{0t}^* + \beta_1 \varepsilon_{0p}^* + \gamma_1 \varepsilon_{0p}^2 \]  \hspace{1cm} (1.27)

where

\[ \varepsilon_{0t}^* = 1 - \varepsilon_{0t} / \varepsilon_{0,XL} \]  \hspace{1cm} (1.28) 

\[ \varepsilon_{0p}^* = 1 - \varepsilon_{0t} / \varepsilon_{0,XL} \]  \hspace{1cm} (1.29)
and $\alpha_1$, $\beta_1$, and $\gamma_1$ are given by

$$\alpha_1 = \frac{n_t(1+n_t)}{4(1+n_t(14+n_t))(1-v^2)}, \quad (1.30)$$

$$\beta_1 = \frac{(1+n_t)(n_p+n_t+2 n_p n_t)v}{4(1+n_p)(1+n_t(14+n_t))(1-v^2)}, \quad (1.31)$$

and

$$\gamma_1 = \frac{n_p(1+n_t(14+n_t-12 v^2))}{4(1+n_p)(1+n_t(14+n_t))(1-v^2)}. \quad (1.32)$$

The non-dimensional strain energy of Folding Mode 2 is given by

$$U_2^* = \alpha_2 \varepsilon_{0p}^* \varepsilon_{0p}^* + \beta_2 \varepsilon_{0t}^* \varepsilon_{0t}^* + \gamma_2 \varepsilon_{0t}^* \varepsilon_{0t}^* \quad (1.33)$$

where $\alpha_1$, $\beta_1$, and $\gamma_1$ are given by

$$\alpha_2 = \frac{n_p(1+n_p)}{4(1+n_p(14+n_p))(1-v^2)}, \quad (1.34)$$

$$\beta_2 = \frac{(1+n_p)(n_t+n_p+2 n_p n_t)v}{4(1+n_t)(1+n_p(14+n_p))(1-v^2)}, \quad (1.35)$$

and

$$\gamma_2 = \frac{n_t(1+n_p(14+n_p-12 v^2))}{4(1+n_t)(1+n_p(14+n_p))(1-v^2)}. \quad (1.36)$$

The preferred folding direction in each case is the mode with lower overall normalized strain energy.

### 1.4. Transient Analysis Methods

To study complex time-dependent deformation modes, finite element method was employed to evaluate the evolution of swelling in different sections of the sheet as a function of time. Solvent absorption in polymers is commonly modeled with Fick’s Second Law [22,29,30], as

$$\frac{\partial c}{\partial t} = D \nabla^2 c \quad (1.37)$$
where $C$ is the solvent concentration and $D$ is the diffusion coefficient. This is analogous to the heat equation where the quantity corresponding to $C$ is the temperature and that corresponding to $D$ is the thermal diffusivity. This allows an equivalent heat transfer model for simulations.

The time-dependent swelling phenomenon and the resulting folding behavior were analyzed using ABAQUS/Standard with equivalent heat transfer and thermal expansion simulations. A heat transfer analysis was performed on a flat sheet to determine how the solvent absorbs through the system. It was assumed that the deformation of the system does not have a large effect on the solvent absorption in the sheet. The results were used to determine how the swelling of each section affects the full deformation mode. A prescribed temperature boundary condition was applied to the top and bottom surfaces of the sheet. Material properties were varied, while upholding the relationships between elasticity and swelling ratio caused by the different levels of cross-linking density, as described by Table 1.1, until the double folding phenomena was replicated computationally. For the analysis, the number of elements was increased to 81,920 and the number of integration points was increased to 18 through the thickness to more accurately simulate the spatial-variant material property distribution.

Simulation of the double folding phenomena causes a computationally ill-conditioned snapping behavior due to a buildup in residual stress. The automatic stabilization algorithm was used to fix this problem in the transient analysis. The automatic stabilization algorithm in ABAQUS/Standard adds artificial damping to the model to stabilize a diverging solution. Viscous damping forces help to oppose periods of high velocity and add overall stability. In all
analyses the energy dissipated was significantly less than the total strain energy in the system. A full mathematical derivation of this algorithm is documented by ABAQUS [26].

1.5. State Diagram Results

1.5.1. Folding direction versus elasticity and swelling strain

Different folding directions were observed depending on the mechanical properties of the XL and PXL sections. Figure 1.2a depicts the two computationally observed folding directions and corresponding simulation results. Material properties used to obtain these simulations are given in Figure 1.3. Figures 1.3b and 1.3c show folding mode maps for a range of material parameters. Figure 1.3b shows the map of folding modes as a function of the normalized swelling mismatch strain for XL, PXL, and NXL sections with elasticity values of $E_{XL}/E_{NXL} = 6.66$ and $E_{PXL}/E_{NXL} = 5.01$. Because the swelling of the XL section is always less than that of the PXL section, only the cases above the 45 degree dashed line were considered. The blue diamonds are simulation results where Folding Mode 1 is preferred at the given values of swelling ratios, and the red dots indicate swelling ratios where Folding Mode 2 is preferred. The points labeled FM1 and FM2, in Figure 1.3b correspond to the parameters used in the simulations shown in Figure 1.3. The solid line shows the boundary between the swelling ratio regions for two different folding modes predicted by the analytical model.

The effect of elasticity of the PXL and XL sections on preferred folding modes was also studied. Figure 1.3b shows the map of preferred folding direction for different values of the Young’s modulus ratios between the XL, PXL, and NXL sections. Because the Young’s modulus of the XL section is always higher than that of PXL section and the Young’s modulus of the PXL
section is always higher than the NXL section, only cases below the dashed 45 degree line and above the dashed horizontal line were simulated. For these simulations swelling strain values of $\varepsilon_{0XL}/\varepsilon_{0NXL} = 0.323$ and $\varepsilon_{0PXL}/\varepsilon_{0NXL} = 0.632$ were used. The solid line shows the boundary between the two modes predicted by the analytical solution.

Figure 1.3a: Steady state simulation results. Stress is given in kPa. Material properties are listed here and given in Figure 1.3b.

Folding Mode 1: $E_{NXL} = 2.32$ MPa, $\varepsilon_{0sNXL} = 0.53$, $c/c_s = 0.07$.

Folding Mode 1: $E_{NXL} = 2.32$ MPa, $\varepsilon_{0sNXL} = 0.53$, $c/c_s = 0.13$.

1.5.2. *The effect of swelling ratio versus the effect of elastic modulus on folding direction*

It was found that the swelling strain has a much larger effect on folding direction than elasticity.

Since the folding direction is governed by which deformation mode yields lower overall strain energy, this effect can be shown by studying the magnitude of the difference in normalized strain energy, \( \text{abs}(U_1^* - U_2^*) \), where \( U_1^* \) and \( U_2^* \) are described by Equations 1.27 and 1.33 respectively.

The average derivative of this value with respect to normalized elasticity, \( \text{abs} \left( \frac{\partial(U_1^* - U_2^*)}{\partial E_{XL}/E_{NXL}} \right) \) or \( \text{abs} \left( \frac{\partial(U_1^* - U_2^*)}{\partial E_{PXL}/E_{NXL}} \right) \), over the range of values studied in the uniform swelling analysis is an order of magnitude smaller than the average magnitude of the derivative with respect to normalized swelling strain, \( \text{abs} \left( \frac{\partial(U_1^* - U_2^*)}{\partial \varepsilon_{0XL}/\varepsilon_{0NXL}} \right) \) or \( \text{abs} \left( \frac{\partial(U_1^* - U_2^*)}{\partial \varepsilon_{0PXL}/\varepsilon_{0NXL}} \right) \). This is also seen computationally. The
derivative of total strain energy with respect to normalized XL elasticity, \( \frac{\partial u^2}{\partial E_{XL}/E_{NXL}} \), and the derivative of total strain energy with respect to normalized XL swelling strain, \( \frac{\partial u^2}{\partial \varepsilon_{0, XL}/\varepsilon_{0, NXL}} \), were calculated computationally by solving for strain energy while varying \( E_{PXL}/E_{NXL} \) or \( \varepsilon_{0PXL}/\varepsilon_{0NXL} \) and numerically differentiating the results. With the base material properties \( E_{XL}/E_{NXL} = 6.66 \), \( E_{PXL}/E_{NXL} = 5.01 \), \( \varepsilon_{0XL}/\varepsilon_{0NXL} = 0.323 \) and \( \varepsilon_{0PXL}/\varepsilon_{0NXL} = 0.632 \), the results show that the derivative with respect to elasticity is also more than an order of magnitude less than the derivative with respect to swelling strain.

The effect of changes in elasticity versus changes in swelling strain can also be seen by studying plots of folding direction versus swelling strain with constant elasticity and plots of folding direction versus elasticity with constant swelling strain. Figure 1.4a shows the division between folding modes obtained computationally for different values of swelling strain and constant elasticity, only cases above the dashed 45 degree line were simulated to uphold realistic material properties due to the level of cross-linking in each material. One line on the plot was made with the base material properties given in the figure heading. The second line was made with \( E_{NXL} \) cut in half. In each case Folding Mode 1 was below the division line and Folding Mode 2 was above the line. Figure 1.4b shows the division between folding modes obtained computationally for different values of elasticity and constant swelling strain, only cases below the dashed 45 degree line and above the dashed horizontal line were simulated to uphold realistic material properties due to the level of cross-linking in each material. One line on the plot was made with the base material properties given in the figure heading. The second line was made with \( \varepsilon_{0NXL} \) increased by 10%. In each case Folding Mode 1 was below the division line and Folding Mode 2 was
above the line. All division lines were made with over 50 simulations each spread throughout the regions shown on the graph.

Figure 1.4a: State diagram showing sensitivity of folding direction to swelling strain. Base state is described by $E_{XL}/E_{NXL} = 6.66$ and $E_{PXL}/E_{NXL} = 5.01$. Each line indicates the division line between Folding Mode 1 (below the line) and Folding Mode 2 (above the line).

Figure 1.4b: State diagram showing sensitivity of folding direction to elasticity. Base state is described by $\varepsilon_{0XL}/\varepsilon_{0NXL} = 0.323$ and $\varepsilon_{0PXL}/\varepsilon_{0NXL} = 0.632$. Each line indicates the division line between Folding Mode 1 (below the line) and Folding Mode 2 (above the line).
Figure 1.4 shows that a large change in $E_{NXL}$ only produces a relatively small change in the swelling strain plot while a relatively small change in $\varepsilon_{0NXL}$ produces a large change in the elasticity plot. Although not shown here, similar plots can be made with a sheet made of brick elements and the analytical solution described in Section 1.3.2. These plots show that the system is much more sensitive to swelling strain than elasticity. Because of this sensitivity, this work focuses on the effect of swelling strain on folding direction instead of the effect of elasticity on folding direction. Additionally, results obtained with shell elements, brick elements and the analytical solution show relatively poor correspondence in plots of folding direction versus elasticity because these plots are much more sensitive to differences in the model.

### 1.5.3. Comparison between shell and brick elements

To test the validity of the shell element model, plots of folding direction versus swelling strain and folding direction versus elasticity were analyzed for a 2.95 mm, by 2.95 mm, by 120 µm sheet. Figure 1.5 shows the division between folding modes obtained computationally with shell and brick elements for different values of swelling strain and constant elasticity, only cases above the dashed 45 degree line were simulated to uphold realistic material properties due to the level of cross-linking in each material. In each case, Folding Mode 1 was below the division line and Folding Mode 2 was above the line. All division lines were made with at least 50 simulations, each spread throughout the regions shown on the graph. Some brick simulations were folded partially in both directions and it was difficult to determine the final preferred folding mode. Best judgment was used while interpreting results and current work is focusing on obtaining more definitive results.
As shown in Figure 1.5 there is a difference between the shell and brick elements. With brick elements, Folding Mode 1 is preferred more often. This is because with shell elements the stress in the thickness direction of the sheet is ignored and the interaction between the XL and NXL material creates stress in this direction and tends to fold the sheet into Folding Mode 1. Plots of folding direction versus elasticity for shell and brick elements do not match as well. As described in Section 1.5.2 the effect of elasticity on folding direction is significantly less than the effect of swelling strain on folding direction. Because of this, any differences in the model affect the elasticity plot much more than the swelling strain plot and also make the elasticity results less significant. Even though the brick elements are more accurate they take several hours longer per simulation on a full 32 mm by 32 mm by 120 µm sheet, so shell elements were used for all other simulations.

Figure 1.5: Folding direction versus swelling strain for shell and brick elements. $E_{XL}/E_{NXL} = 6.66$ and $E_{PXL}/E_{NXL} = 5.01$. Each line indicates the division line between Folding Mode 1 (below the line) and Folding Mode 2 (above the line).
1.6. Transient Analysis Results

1.6.1. Material property selection

It should be noted that only particular ranges of material properties lead to double folding behavior in the transient simulation. These material properties include diffusion rates of solvent, maximum swelling ratios, and the elasticities of each section. In the current simulation, we selected the material properties such that double folding occurs while maintaining the relationship between material properties due to the level of cross-linking in each material described by Table 1.1.

To find material properties that lead to double folding in the transient simulation, an approximate one-dimensional analytical solution was developed that can predict solvent concentration in the material as a function of time at each location through the thickness of the sheet. It was assumed that the XL, PXL and NXL material sections only absorbed solvent from the side of the sheet facing the liquid and that each material is infinitely long in each dimension perpendicular to the thickness direction. The concentration at the side of the sheet exposed to toluene is kept at fully saturated and there is no diffusion of solvent at the boundary between the halves of the sheet. Figure 1.6 gives a description of the system for each material.
where \( i \) is an index representing the XL, PXL or NXL material, \( x_i \) and \( x \) is the dimension shown in Figure 1.6 in material \( i \), \( C_i \) is the solvent concentration in material \( i \), \( D_i \) is the diffusion coefficient of material \( i \), \( t \) is time, \( L \) is the thickness of the material section (\( L = 0.6\mu m \) for all materials), and \( C_s \) is the fully saturated concentration.

A one-dimensional version of Equation 1.37 was used to model the solvent diffusion. The equations that describe the concentration of solvent in each material as a function of \( x_i \) and \( t \) is given by

\[
\frac{\partial C_i}{\partial t} = D_i \frac{\partial^2 C_i}{\partial x_i^2} \tag{1.38}
\]

\[
C_i(x = 0, t \geq 0) = C_s H(x), \tag{1.39}
\]

\[
\frac{\partial C}{\partial x_i}(x_i = L, t) = 0, \tag{1.40}
\]

\[
C_i(x_i, t) = 0, \tag{1.41}
\]

\[
t \geq 0, \tag{1.42}
\]

and

\[
0 \leq x_i \leq L, \tag{1.43}
\]
where $H(x)$ is the Heaviside Step Function. Using separation of variables, it can be shown that the solution to Equations 1.38-1.43 is given by

$$c_i(x_i, t) = \sum_{n=0}^{\infty} \frac{4 \epsilon (2n-1)^2 \pi^2 t}{4L^2} \left( \cos\left(\frac{(2n-1)\pi}{2}\right) - 1 \right) \sin\left(\frac{(2n-1)\pi x}{2L}\right).$$  \hspace{1cm} (1.44)

Values of diffusion coefficient $D$ for each material section were found such that the solvent concentration at $x = L$ reaches ninety nine percent of saturation at the same time as the actual double folding sheets finish deforming. Given the state diagram in Figure 1.3b, the saturation swelling strain $\varepsilon_{0s}$, as described by Equation 1.2, was selected for each material such that the sheet favors Folding Mode 2 at the end of the simulation, and there is a large difference between the swelling strain in the NXL and PXL material halfway though the thickness of each material section at fifty percent of the time it takes for the material to reach ninety nine percent of full saturation. While this is not an exact calculation, it offers a good starting point to find realistic material properties that produce double folding.

### 1.6.2. Transient Simulation Results

The double folding phenomena can be analyzed by studying what causes the specimens to change from the blue to red regions of Figures 1.3b or 1.3c. In addition to the uniform swelling analysis, the double folding phenomenon was studied using a transient analysis. For this analysis elasticity was held constant during the simulation. While one could have changed the elasticity of each material throughout the simulation, as described in Sections 1.5.2 and 1.6.3, it was found that changing elasticity did not have a significant effect on the deformation mode of the simulation.
For the double folding simulation, elasticities of $E_{XL} = 20.00$ MPa, $E_{PXL} = 15.00$ MPa, and $E_{NXL} = 5.00$ MPa, swelling ratios of $\varepsilon_{0sXL} = 0.057$, and $\varepsilon_{0sPXL} = 0.13$, and $\varepsilon_{0sNXL} = 0.177$ and diffusion coefficients of $D_{XL} = 8e-3$ m$^2$/s, $D_{PXL} = 1.5e-3$ m$^2$/s, and $D_{NXL} = 1.21e-4$ m$^2$/s were used.

Figure 1.7a below shows experimental time-lapse images of the double folding phenomena and Figure 1.7b shows corresponding simulation results. Stress values are given in kPa.

Figure 1.7a: Experimental double folding images. Adapted from Design, fabrication, and application of stimuli-responsive hydrogel actuators (p. 205), by P. Yuan, 2014, Available from IDEALS. Copyright 2014 by Peixi Yuan, Adapted with permission.

Figure 1.7b: Computational double folding images showing simulation time. Stress is given in kPa.
In order to understand what causes the double folding phenomena a plot of swelling strain halfway through the thickness of each material section is shown in Figure 1.8a. Figure 1.8b shows the total strain energy throughout the simulation. The labels A-F in Figures 1.8a and 1.8b refer to the computational times shown in Figure 1.7b.

Figure 1.8a: Swelling strain of each material during the double folding phenomena. Labeled points are shown in Figure 1.7b.

Figure 1.8b: Strain energy during double folding. Labeled points are shown in Figure 1.7b.
1.6.3. Effect of elasticity on double folding

This sensitivity of folding direction to swelling ratio as described in Section 1.5.2 is also observed in transient simulation results. Horkay et al. [31] tested the elasticity of different types of PDMS and toluene mixtures and found that swelling in toluene lowers the elasticity of PDMS by about a factor of three. Starting with our base elasticity values used in the double folding simulation, the double folding mechanism is still observed if the NXL material is increased by a factor of four with the other elasticities held constant. However, the double folding phenomena is much more sensitive to any changes in saturated swelling strain.

1.7. Discussion

1.7.1. The effect of material properties on folding direction

Figures 1.3b and 1.3c show that the steady state numerical and analytical models produce similar results. The difference between the two models is significantly greater when elasticity is varied (Figure 1.3c). As discussed in Sections 1.5.2 and 1.6.3, close analysis of the analytical solution shows that the transition between the two folding modes is much more sensitive to swelling strain than to elasticity. Small changes in swelling ratio will drastically shift the analytical cutoff between the two folding modes shown in Figure 1.3c. Because of this sensitivity, any assumptions would likely affect the results shown in Figure 1.3b more than those in Figure 1.3c.

By studying the analytical model, the steady state results can be better understood. Equations 1.27-1.36 show that the folding direction is a function of the difference between the swelling strain in the top and bottom layer of the sheet. Specifically, for the values of elasticity used in Figure 1.3b, increasing the difference between the swelling strain transverse to the XL lines and
the swelling strain of the PXL material, \( \text{abs}(\varepsilon_{ot} - \varepsilon_{0PXL}) \), will make Folding Mode 1 preferred. Conversely increasing the difference between the swelling strain parallel to the XL lines and the swelling strain of the PXL material, \( \text{abs}(\varepsilon_{op} - \varepsilon_{0PXL}) \), will make Folding Mode 2 preferred. To further understand the results, a plot of swelling strain transverse and parallel to the XL lines \( \varepsilon_{0t} \) and \( \varepsilon_{0p} \) as a function of the swelling strain of the XL material \( \varepsilon_{0XL} \) is shown in Figure 1.9a for swelling strain values around the analytical cutoff between folding modes in Figure 1.3b. As shown in the figure, increasing \( \varepsilon_{0XL} \) will decrease \( \text{abs}(\varepsilon_{op} - \varepsilon_{0PXL}) \), and increase \( \text{abs}(\varepsilon_{ot} - \varepsilon_{0p}) \), which is why increasing \( \varepsilon_{0XL} \) can cause the specimens to change from Folding Mode 2 to Folding Mode 1 in Figure 1.3b. Increasing \( \varepsilon_{0XL} \) will also lower the strain difference in the XLB making the strain difference in the NXLB the driving force behind folding. Increasing \( \varepsilon_{0PXL} \) with other properties held constant will increase \( \text{abs}(\varepsilon_{op} - \varepsilon_{0PXL}) \), and decrease \( \text{abs}(\varepsilon_{ot} - \varepsilon_{0PXL}) \), changing the preferred folding direction from Folding Mode 1 to Folding Mode 2. This makes the strain difference in the XLB the driving force behind folding.

The analytical solution can also help explain results in Figure 1.3c. At a point near the transition between Folding Mode 1 and Folding Mode 2, increasing the values of \( n_t \) or \( n_p \) (where \( n_t = E_t / E_{PXL} \), and \( n_p = E_p / E_{PXL} \) as previously defined) will make folding preferred transverse or parallel to the lines respectively. That is because if the Young’s modulus is higher in one direction on top of the sheet it takes extra energy to prevent any bending in that direction. Figure 1.9b shows a plot of \( E_t \) and \( E_p \) as a function of \( E_{XL} \) for elasticity values around the analytical cutoff between folding modes in Figure 1.3b.
This figure shows that increasing $E_{XL}$ will increase $n_p$ more than $n_t$ and correspondingly cause specimens to change from Folding Mode 1 to Folding Mode 2. Understanding why increasing
The steady state analysis can show which mechanical characteristics cause specimens to fold in each direction. The analysis can be used to analyze sheets with different folding modes. The model can also be used to design and analyze specimens that experience double folding. It is clear that in order for a sheet to experience double folding it must move from blue to red on Figure 1.3b or 1.3c.

### 1.7.2. Complex folding modes

It is known from Figure 1.8a that at the beginning of the simulation the PXL and XL materials have almost the same swelling strain and the swelling strain of the NXL material is much higher. This is because the NXL absorbs solvent significantly faster than the other materials. As the simulation continues, the NXL material reaches saturation the fastest and the swelling strain in the PXL material approaches the swelling strain in the NXL material. This changes the preferred folding direction from Folding Mode 1 to Folding Mode 2 causing the double folding observed experimentally.

An important feature of the double folding is the quick snap from Folding Mode 1 to 2. This is seen in Figures 1.7a and 1.7b, between Images F and G. The snap is faster in the computational results, likely because the computational results do not account for softening of each material
during folding. During this deformation mode there is not enough energy to bend the whole sheet while it is still partially rolled into Folding Mode 1, but eventually the stress field changes enough to cause the sheet to fully unroll and then snap into Folding Mode 2. This is better understood by analyzing Figure 1.8b. As the sheet folds the strain energy increases. The sheet unfolds and eventually snaps into Folding Mode 2 releasing energy extremely quickly. Afterward there is a slight increase in energy as it moves into Folding Mode 2.

Quick actuation of a soft polymer is a difficult task. In the past, researchers have studied polymer dome-like structures that exhibit a snap-through characteristic as they are inverted [13,32,41,42]. This unique double folding system uses a buildup in residual stress to achieve actuation.

To further test the model, several specimens that fold into more complex folding modes were built. The deformations are much more complex and more difficult to replicate. However, after some modification of material properties, they were replicated with a computational model. The results are shown in Figure 1.10 below, and the necessary material properties are listed in the caption below the figure.
Automatic stabilization is used for these simulations, but like before, the energy dissipated was at least two orders of magnitude less than the total energy in the system.

1.8. Conclusions

Mechanistic models can be used to design and analyze polymer systems fabricated with gradients of cross-linking density. Even with a relatively simplistic model, folding direction and other complex deformation modes can be predicted and replicated accurately. The model can also predict quick actuation and further work will focus on the analysis of various fast-actuating...
modes. This will allow researchers to develop polymer systems for a variety of applications. Shapes can be designed using this model for small-scale fabrication and micro mechanical machines can be designed and built efficiently.

1.9. Future Work

Future work will focus on developing other systems that actuate quickly or using the system as a fabrication procedure. Work will focus on building a circular dome structure that experiences limit point buckling. The system will also be investigated as a fabrication procedure for microfluidic devices at small scales. Overall, a wide variety of deformation modes will be investigated.

The model will be refined by a more accurate characterization of material properties during the swelling process. The absorption of solvent into the material will be modeled and the evolution of swelling strain and elasticity will be characterized as a function of saturation percentage. The material property characterization will be carried out computationally and experimentally with atomic force microscopy or similar experimental techniques. In addition to mechanistic modeling, structure optimization algorithms, will be investigated as a powerful tool to help with design of complex shapes for a variety of applications. With this more robust modeling, a wide variety of structures will be designed and optimized, easily making the system an even more powerful tool.
CHAPTER 2: COMPUTATIONAL ANALYSIS OF A DOME SHAPED BIOLOGICAL MACHINE

Other research contributors: Amit Madhukara, Michael Grigolab, Donghai Gai, K. Jimmy Hsia

2.1. Introduction

Recent research at the University of Illinois has focused on developing walking [33] and swimming [34] biological machines called bio-bots that are powered by cells. These systems give a better understanding of the emergent behavior of cells and have important potential applications for in vivo drug delivery or chemical sensing. These biological systems have been powered by mouse cardiomyocytes [33,34], which contract spontaneously.

This work investigates a dome-like shape for potential use as a different scaffold for these bio-bots, called a hopper. The dome will invert due to cell forces and then automatically flip back into its original configuration due to the material’s viscoelasticity. During dome inversion the structure also actuates quickly as it buckles and snaps though to its secondary configuration.

A majority of sections and figures except Sections 2.3.1, 2.4, 2.5.2, 2.6.1, and 2.7 and Figures 2.2, 2.4, 2.9, and 2.11 are reprinted from “Bistable characteristics of thick-walled axisymmetric domes,” by A. Madhukar, D. Perlitz, M. Grigola, D. Gai, and K. J. Hsia, 2014, Int. J. Solids Struct, In Press, 1-8. Copyright 2014 by Elsevier Limited. Reprinted with permission.

a: Contributed significantly to research and develop the model. Helped post process results. Independently made Figures 2.1,2.3 and 2.5. Post processed results on Figure 2.6, 2.7, 2.8, and 2.10, Table 2.3 and Equation 2.8. Did research for part of the literature review. First author on publication.
b: Performed experiments related to the computation.
c: Helped develop the computational model.
This quick actuation has been used as mechanical switches [35,36]. This snapping behavior is also seen in biological systems such as the Venus flytrap [37,38]. Past mechanics research in this area has focused on stability and deformation of thin domes [39,40]. Brinkmeyer et al. [41] and Santer [42] investigated the stability characteristics of domes to identify when the domes snap back automatically to their original configurations. The work described here models thick domes where the stress cannot be ignored in any direction. Using finite element analysis, a model is developed that can predict the stability of a dome’s secondary state, and predict the force necessary to invert the system. This will allow for the optimal design of a bio-bot system. In this work, the model is discussed in detail and the experimental work needed to build the dome-shaped bio-bot is discussed.

2.2. Problem Definition

To develop a bio-bot that can be powered by cells, a mechanistic model was developed that can predict stability characteristics and the force needed to actuate the machine. Figure 2.1 below describes the input geometry.
The variable $\delta$ is the displacement of the outer ring of the dome. The system has a constant cross-sectional thickness and a hole at the top of the dome. It was assumed that the material was linear elastic and isotropic. Finite element analysis was used to find force versus displacement and energy versus displacement for the geometric parameters described in Figure 2.1, Young’s Modulus, $E$ and Poisson’s Ratio, $\nu$.

The Buckingham Pi Theorem was used to create non-dimensional variables and reduce the number of parameters governing the system [43]. The analysis takes the form

$$E = f (e, \nu, H, L, t, r_h, \delta)$$

(2.1)

where $E$ is the energy in the system, $e$ is the elasticity, $\nu$ is the Poisson’s ratio, $H, L, t,$ and $r_h$ are the geometric parameters described by Figure 2.1, and $\delta$ is the displacement of the outer ring of.

the dome. Table 2.1 gives the dimensions of each variable written in terms of mass \([m]\), length \([L]\), time \([T]\), and temperature \([\Theta]\).


<table>
<thead>
<tr>
<th></th>
<th>(E)</th>
<th>(e)</th>
<th>(\nu)</th>
<th>(H)</th>
<th>(L)</th>
<th>(t)</th>
<th>(r_h)</th>
<th>(\delta)</th>
</tr>
</thead>
<tbody>
<tr>
<td>([m][L]^{-2}[s]^{-2})</td>
<td>([m][L]^{-1}[T]^{-2})</td>
<td>[-]</td>
<td>([L])</td>
<td>([L])</td>
<td>([L])</td>
<td>([L])</td>
<td>([L])</td>
<td></td>
</tr>
</tbody>
</table>

Using these variables the matrix of dimensions is given by

\[
\begin{bmatrix}
E & e & \nu & H & L & t & w & \delta \\
L & 2 & -1 & 0 & 1 & 1 & 1 & 1 \\
m & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\
T & -2 & -2 & 0 & 0 & 0 & 0 & 0 \\
\theta & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}.
\]

The rank of the matrix in Equation 2.2 is 2 meaning there are two variables with independent dimensions and 6 non-dimensional Pi groups can be constructed. Using \(L\) and \(e\) to non-dimensionalize each parameter, 6 pi groups are developed.

Table 2.2: Non-dimensional dome variables.

<table>
<thead>
<tr>
<th>(E^*)</th>
<th>(\nu^*)</th>
<th>(H^*)</th>
<th>(t^*)</th>
<th>(r_h^*)</th>
<th>(\delta^*)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(En e^{-1} L^{-3})</td>
<td>(\nu)</td>
<td>(H L^{-1})</td>
<td>(t L^{-1})</td>
<td>(r_h L^{-1})</td>
<td>(\delta L^{-1})</td>
</tr>
</tbody>
</table>

From the Buckingham Pi Theorem the system can be expressed as

\[
E^* = f(\nu^*, H^*, t^*, r_h^*, \delta^*).
\]

The relationship
\[ F = f(e, \nu, H, L, t, r_h, \delta) \]  

(2.4)

was also analyzed, where \( F \) is the force applied to the outer rim of the dome throughout its motion. Using a similar analysis as above, force can be non-dimensionalized by \( F^* = F e^t L^{-2} \) and thus the system is given by

\[ F^* = f(v^*, H^*, t^*, r_h^*, \delta^*). \]  

(2.5)

As described in Section 2.5.2 the whole size \( r_h^* \) had little effect on the results for small hole radius, so the hole size is not discussed in detail in this work. For most simulations, Poisson’s ratio was kept at 0.49, the literature value for Polydimethylsiloxane (PDMS) [18], which was used to construct all domes.

2.3. Methods

Finite element analysis (FEA) is often utilized in the study of both bifurcation and limit point buckling [44]. Bifurcation buckling occurs when the equilibrium solution to the mechanical system divides into multiple paths. In limit point buckling, a system reaches a mechanical configuration at which further deformation yields an unstable state, and the system is forced to snap into a secondary equilibrium state. Limit point buckling describes the type of deformation seen by the dome as it snaps though into its inverted configuration.

2.3.1. Linear FEA

One approach to analyzing buckling systems is eigenvalue analysis [26]. Eigenvalue analysis is a linear finite element technique commonly applied to bifurcation buckling. It is often beneficial because it is computationally inexpensive, however its accuracy is limited in nonlinear problems.
Linear eigenvalue analysis has been developed for use in ABAQUS, and a full mathematical derivation is available [26]. Eigenvalue analysis involves solving the equation:

\[(K + \lambda_i)v_i = 0\]  

(2.6)

where \(K\) is the base state stiffness matrix, \(K_\Delta\) is the differential stiffness matrix, \(\lambda_i\) is an eigenvalue associated with the reference load, and \(v_i\) is the corresponding eigenvector. The differential stiffness matrix is a function of element type, geometry, and the applied reference loads. This matrix relates membrane stresses to lateral deflections in the system. The critical buckling load is calculated by multiplying the eigenvalue by the initial reference load and \(v_i\) represents the deformation mode associated with each eigenvalue. Solving Equation 2.6 yields \(\lambda_i\) and \(v_i\) such that no net stiffness resists the deformation described by the buckling mode \(v_i\) [45].

The eigenvalue model used 8 node quadratic shell elements with 5 degrees of freedom per node. The final swept mesh can be seen in Figure 2.2a. A pinned boundary condition was used on the bottom outer ring of the dome and a downward reference force was applied around the hole on the top of the dome. The model was used to identify the force required to cause local buckling at the top of the dome. The deformation mode is shown in Figure 2.2b.
Although linear analysis is computationally inexpensive, nonlinear FEA is required to analyze large deformation buckling problems or to study post-buckling behavior of linear systems [45]. Common nonlinear FEA methods used to study buckling systems include arc length method and static damping method, both of which are described here. For these analyses, three-dimensional
quadratic tetrahedral elements were used to model the geometry described in Figure 2.1. The center of the hole at the top of the dome was pinned in each direction and an upward displacement boundary condition was applied to the outer rim of the dome so it is fully inverted. A mesh convergence study was also performed to ensure accuracy of the results. Figure 2.3 shows the mesh used for all nonlinear finite element models.

Finite element analysis was used to find force versus displacement at the end of the dome as it inverts and energy versus displacement curves for a variety of dome geometries. Given the energy versus displacement curves, the stability of domes can be analyzed to help design an efficient biological machine.

Common nonlinear FEA methods for analyzing buckling systems are known as arc length methods. One arc length method is the “modified Riks method”, which has been implemented in
ABAQUS and is documented [26]. Riks method has been used to study a variety of buckling problems, including post-buckling behavior of reinforced plates [46] and limit point buckling of steel domes [47].

The modified Riks method assumes the load at each solution increment is related to the magnitude of the full load by a factor $\lambda$ [26]. Modified Riks solves for the relationship between $\lambda$ and the displacement, $u$. At each increment, the tangential stiffness matrix is used to find the line tangent to the $\lambda$-$u$ curve at the current solution point. The tangent line is traversed a distance related to the current arc length, which is initially specified by the user, and adjusted adaptively in ABAQUS. The algorithm then looks for equilibrium in the plane that passes though this new point and is perpendicular to the tangent line.

Static damping analysis is another approach that uses dashpots to prevent divergence in the buckling system [48]. The problem is solved using Newton-Raphson iterations as in a geometrically nonlinear static analysis. The difference is that at each Newton-Raphson iteration, dashpots help stabilize the system by adding small, viscous damping forces. These forces oppose the high velocity motion encountered during buckling. Damping forces are calculated by

$$F = \mu M \frac{u}{\Delta t}$$

(2.7)

where $F$ is the force matrix, $\mu$ is the damping coefficient, $M$ is the artificial mass matrix, $u$ is the displacement matrix, and $\Delta t$ is the current time step. The model is considered valid if the total energy dissipated by artificial damping is significantly less than the total elastic strain energy. Dashpots can be added to each node manually or automatically to the whole system with the ABAQUS “automatic stabilization” option [26]. This dashpot method has been used by
Hoveidae et al. [49] to study the buckling behavior of restrained braces used in buildings, and Becque et al. [48] to study the buckling of stainless steel I columns. A full description of the static damping method is documented by ABAQUS [26].

2.3.3. Experimental Methods

The model was verified experimentally by constructing PDMS domes from molds made of ball bearings. The stability characteristics of these domes were compared to the stability characteristics predicted from finite element analysis. Additionally, the force versus deflection curve of a rubber-like dome was measured experimentally and the results were compared to curves obtained with finite element analysis. These results are not described here but Madhukar et al. [32] describes these results in detail.

2.4. Linear Results

An eigenvalue analysis was used to analyze the deformation mode seen in Figure 2.2b, Figures 2.4a and 2.4b show how $H/L$ and $t/L$ relate to the nondimensional force required to cause this local buckling. The force needed to cause snap through buckling in a Riks analysis is overlaid on each graph. All domes had an upper hole with a radius of 8.3e-5m. Figure 2.4a was obtained with $t/L = 0.083$, and Figure 2.4b was obtained with $H/L = 0.333$. These simulations were obtained with a Poisson’s ratio, $\nu$, of 0.4.
2.5. Nonlinear results

Using nonlinear finite element methods, individual domes were simulated as they inverted into their secondary configuration. Figure 2.5a shows computational results during the simulation. Using these simulation results, plots of normalized force versus normalized displacement were obtained for a variety of dome geometries. An example of one of these curves is shown in Figure

Figure 2.4a: Force versus H/L Plot for Eigenvalue Analysis and Modified Riks Method. $t/L = 0.083$.

Figure 2.4b: Force versus $t/L$ Plot for Eigenvalue Analysis and Modified Riks Method. $H/L = 0.333$. 
2.5b. Differentiating the curve in Figure 2.5b produces a plot of normalized energy versus displacement, shown in Figure 2.5c.


Figure 2.5c: Nondimensional energy versus nondimensional displacement. Labeled points correspond to simulation images in Figure 2.5a. Reprinted from “Bistable characteristics of thick-walled axisymmetric domes,” by A. Madhukar, D. Perlitz, M. Grigola, D. Gai, and K. J. Hsia, 2014, *Int. J. Solids Struct, In Press*, p. 4. Copyright 2014 by Elsevier Limited. Reprinted with permission.
The stability of this system can be characterized by the energy well $E_d^*$ shown in Figure 2.5c. If there is no energy well the system is mono-stable and upon inversion the dome immediately flips back into its original configuration. At large values of $E_d^*$ the system is bi-stable; it has a secondary energy state and after inversion the dome stays in its inverted state. At low positive values of $E_d^*$ the dome is pseudo-bistable and will automatically flip back into its secondary configuration due to its viscoelasticity. This phenomenon is not investigated in detail here but is described in past work.

To find how the system is affected by changes in geometric properties, the energy well $E_d^*$ was calculated for various geometries. The results were fit to a surface equation, which is given below. Figure 2.6 shows a plot of this relationship.


<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Value $\times 10^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$b_{00}$</td>
<td>0.0175</td>
</tr>
<tr>
<td>$b_{10}$</td>
<td>1.239</td>
</tr>
<tr>
<td>$b_{01}$</td>
<td>-0.392</td>
</tr>
<tr>
<td>$b_{20}$</td>
<td>-8.19</td>
</tr>
<tr>
<td>$b_{11}$</td>
<td>-2.699</td>
</tr>
<tr>
<td>$b_{02}$</td>
<td>1.167</td>
</tr>
<tr>
<td>R-squared</td>
<td>0.9614</td>
</tr>
<tr>
<td>Number of points</td>
<td>91</td>
</tr>
</tbody>
</table>
\[ Ed^* = b_{00} + b_{10} \frac{t}{L} + b_{01} \frac{H}{L} + b_{20} \left(\frac{t}{L}\right)^2 + b_{11} \frac{H \cdot t}{L^2} + b_{02} \left(\frac{H}{L}\right)^2 \]  

(2.8)


It is important to note that this relationship is only valid for values of \( H/L \) and \( t/L \) that were simulated. Domes with positive \( Ed^* \) and low thickness were not simulated. The simulation points are given with an * in Figure 2.7 below.
2.5.1. Testing the non-dimensional system

To test the non-dimensional system described by Equations 2.3 and 2.5 multiple domes with equal values of $v^*$, $H/L$, $t/L$, $r_b/L$, and $\delta/L$ were analyzed. Figure 2.8 below shows plots of Force versus Displacement and Energy versus Displacement for two domes, one double the size of the other, meaning they have the same non-dimensional input parameters.


As shown, the Pi groups effectively non-dimensionalize the system and consequently reduce the number of variables needed to study the system. These simulations were obtained with a Poisson’s ratio, \(\nu\), of 0.4.

2.5.2. Effect of hole radius \(r_h\)

The effect of hole radius \(r_h\) was quantified by finding the depth of the nondimensional energy well \(E_d^*\) for various hole diameters. These simulations were obtained with a Poisson’s ratio, \(\nu\), of 0.4. This is plotted in Figure 2.9, the geometric parameters used in these simulations are described in the figure caption.

![Figure 2.9: Nondimensional energy well depth versus hole radius.](image)

As shown, the hole produces a relatively small change in \(E_d^*\) for values of \(r_h/L\) less than 0.045. Because of this, hole size is not considered in this analysis.

2.5.3. Static Damping Method
In Figure 2.10, the energy-displacement curves obtained with the modified Riks method are compared with those obtained with the static damping method. The boundary conditions, mesh, and element type for this analysis are described in Section 2.2, and the geometry is defined by $H/L = 0.43$ and $t/L = 0.083$. Dashpots were connected from each node on the bottom outer rim of the dome to ground. We applied three dashpots to each node, one for each Cartesian direction, and gradually increased the damping on each dashpot until the divergent static analysis converged. This analysis used a damping coefficient of $1e-8 \text{ N-s/m}$ for each dashpot. The total elastic energy dissipated by damping was four orders of magnitude lower than the total energy in the system. To quantify the difference between the two solutions we calculated the root mean square deviation (NRMSD), normalized by the range of dimensionless energy values $(E_{d_{\max}} - E_{d_{\min}})$. The NRMSD for the energy versus displacement curves in Figure 2.10 is 0.0335%. For additional comparison we calculated the NRMSD for domes with 50 different geometries. We did not find the ideal damping coefficient for each individual dome, which would have ensured the highest level of accuracy; however, we were still able to obtain a maximum NRMSD of 5% and an average NRMSD of 2.95%.
Comparing solutions found with both Riks method and damping method is important for verifying their solutions. As shown in Figure 2.10 the modified Riks method and static damping method provided very similar results for the various geometries tested. For higher accuracy, the damping method still necessitates finding an artificial damping coefficient for each new geometry such that the energy dissipated is negligible, yet is sufficient to give a convergent solution. Riks method does not demand this parameter, and is also more common in studying large deformation buckling systems [50]. However, for certain geometric configurations, Riks method may not converge. The static damping method, or even an eigenvalue analysis, may then be called upon to study the system.

Figure 2.10: Energy versus displacement plot for Modified Riks Method and Static Method with Damping. \( H/L = 0.43 \) and \( t/L = 0.083 \). Reprinted from “Bistable characteristics of thick-walled axisymmetric domes,” by A. Madhukar, D. Perlitz, M. Grigola, D. Gai, and K. J. Hsia, 2014, *Int. J. Solids Struct., In Press*, Supplemental p. 4. Copyright 2014 by Elsevier Limited. Reprinted with permission.
2.6. Discussion

2.6.1. Linear Analysis

Using an eigenvalue analysis one can find the relationship between geometric properties and the force necessary to cause the local buckling seen in Figure 2.2b. Figures 2.4a and 2.4b, obtained with an eigenvalue analysis, show that the parameters $H/L$ and $t/L$ are proportional to the amount of force necessary to produce downward deformation around the center of the dome. While the deformation states predicted by eigenvalue analysis and Riks method are not equivalent, there are important relationships between the two. The eigenvector shown in Figure 2.2b is a possible preliminary deformation state, beyond which a small force may lead to snap-through buckling. The two analyses also differ in their boundary conditions, which are described in Sections 2.2 and 2.3.1. With different deformation modes and boundary conditions, the Riks method and Eigenvalue curves shown in Figures 2.4a and 2.4b are not equivalent. However, the slope and force values show some relation for both sets of curves. Because of these similarities, an eigenvalue analysis can be used to help design a dome that is resistant or susceptible to large deformation buckling. This is beneficial because eigenvalue analysis is more computationally inexpensive than Riks method, and therefore may be useful for large or complex geometries.

2.6.2. Nonlinear Analysis

Figure 2.6 shows that increasing $H/L$ and $t/L$ causes $Ed^r$ to increase, consequently increasing the stability of the dome. From these results one can design a system with a desired stability level. The force needed to invert each dome can also be found for each individual dome. In Madhukar et al. [32] these results are verified by comparing computational results to prototyped PDMS
domes. From these results an optimal bio-bot can be designed that flips due to cell forces and later automatically flips back to its original position.

2.7. Conclusions and Future Work

Using this model an effective biological machine can be designed. The force necessary for inversion and the dome’s stability characteristics can be predicted from input geometries. Therefore, a dome can be designed that inverts due to cell forces and snaps back automatically. Still a more robust model is possible, accounting for the viscoelasticity of the system, which would allow more precise prediction of pseudo bi-stability and better prediction of the system’s deformation. Future work will focus on implementing viscoelasticity in the model and using the model to design various biological systems.

Mouse myoblasts (C2C12 cells) have been grown on the domes to experimentally determine optimal conditions to power the bio-bot. These domes were built by sequentially curing PDMS on top of ball bearings and then using a sharp hole punch to remove the dome from the bearing. Both sides on the dome surface were functionalized with fibronectin and cells were plated on both sides of the dome. After two days of incubation the media was changed to Dulbecco’s Modified Eagle’s Medium (DMEM) supplemented with 10% Fetal Bovine Serum (FBS). Some myotubes were successfully grown on the surface of the bio-bots. The beginning of myotube formation can be seen in Figure 2.11.
Future work will focus on developing a precise fabrication technique to build the bio-bot. Possible fabrication techniques include stereolithography or injection molds. Cells will be grown on the domes and an electric shock will be used to power the system. From the finite element model, a bio-bot will be able to be designed that can store energy and actuate quickly.

Figure 2.11: Myotubes beginning to form on a PDMS bio-bot.
References


