

A Dodecahedral Model for Alveoli

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Abstract

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Part 1

Introduction

Injuries that occur after blast waves impact a soldier wearing Personal Protective Equipment (PPE) or that occur after non-penetrating ballistic projectiles impact a soldier wearing PPE are referred to as Behind Armor Blunt Trauma (BABT). The kinetic energy from such impacts is absorbed by a soldier's PPE, and by the bony and soft tissues of the soldier beneath. Standards have been written by which PPE's have been designed to since 1972. Verification is through experiments where, typically, a suit of body armor is placed over a 'body' subjected to a ballistic impact from a projectile fired by a weapon, all in accordance with a standard. Current practice is to use clay (usually Roma Plastilina No. 1 clay) as a surrogate for the human body in these tests. A principle objective of an internal Army Research Laboratory–Weapons and Materials Research Directorate (ARL-WMRD) project, *Modeling Large Deformations and Stress Wave Mechanics in Soft Biological Tissue*, is to develop accurate material models for the human body that are also efficient in their finite element implementation, thereby facilitating the study BABT. This is a 6.1 research project whose hand-off to a 6.2 development team at project's end will aid Army engineers in their design of improved PPE by allowing them to run in-silico BABT tests to complement their actual in-field experiments.

The ARL-WMRD *Modeling Large Deformations and Stress Wave Mechanics in Soft Biological Tissue* project has three primary objectives: *i*) new material models, *ii*) new experiments, and *iii*) new trauma metrics. Lung has been selected as the soft tissue of interest for this study. What are sought are models and metrics whose parameters are physical and unique, and whose numeric implementation will be efficient and stable. Continuum thermodynamic models for lung tissue and a trauma metric are being developed (Clayton & Freed [1, 2] and this document). The work done under this sub-project, *A Dodecahedral Model for Alveoli*, complements its parent project, *Modeling Large Deformations and Stress Wave Mechanics in Soft Biological Tissue*, with regards to the first and third objectives of this ARL-WMRD program. The models being developed are expected to be improvements over those currently supplied by LS-Dyna in their materials library that, e.g., have been used to study shock waves traversing a human torso not wearing body armor, as shown in Fig. 1.1.

BABT occurs at the microscopic level of alveoli, which make up the parenchyma, i.e., the spongy tissue of lung that comprises around 90% of lung by volume, cf. Fig. 1.2, there being some 500 million alveoli in a lung. Most damage occurs just beneath the visceral pleural, as seen in Fig. 1.3, and is a consequence of the large disparity in wave speeds between solid tissues ($\sim 1,500$ m/s) and the spongy parenchyma ($\sim 30\text{--}40$ m/s) [4]. The objective of this work is to develop a mechanistic multi-scale model capable of describing the deformation and damage that occur at an alveolar level, caused by a shock wave traveling through the parenchyma, induced through either a blast or a ballistic impact to a soldier's PPE. In-silico experiments done using this microscopic model are to be used to 'inform' our macroscopic model in those areas where actual lung experiments are difficult if not impossible to perform.

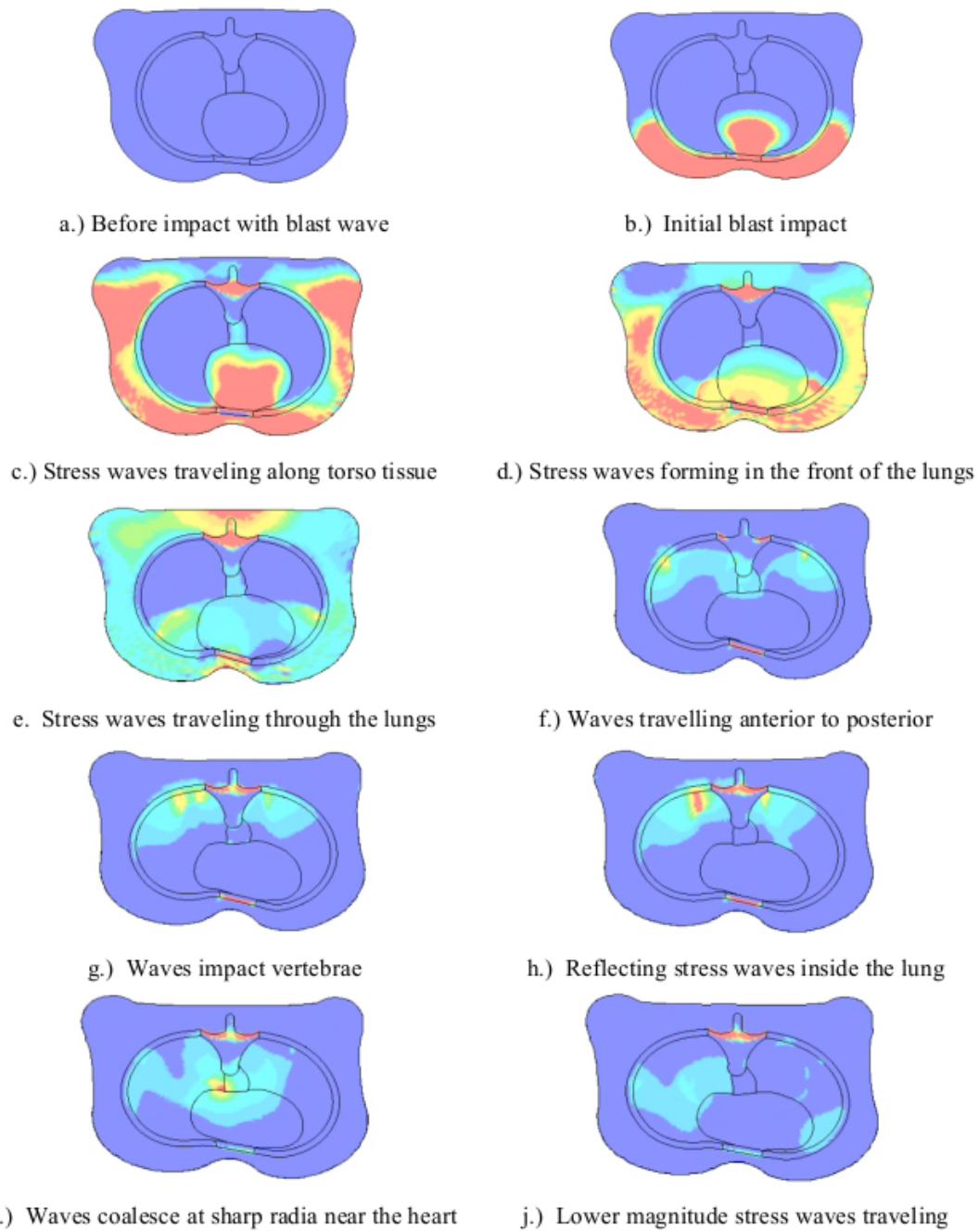


Figure 1.1: Finite element analysis done using LS-Dyna to model shock waves traversing a cross-sectional slice of a human torso. Material models from the LS-Dyna library of available models were used [3].

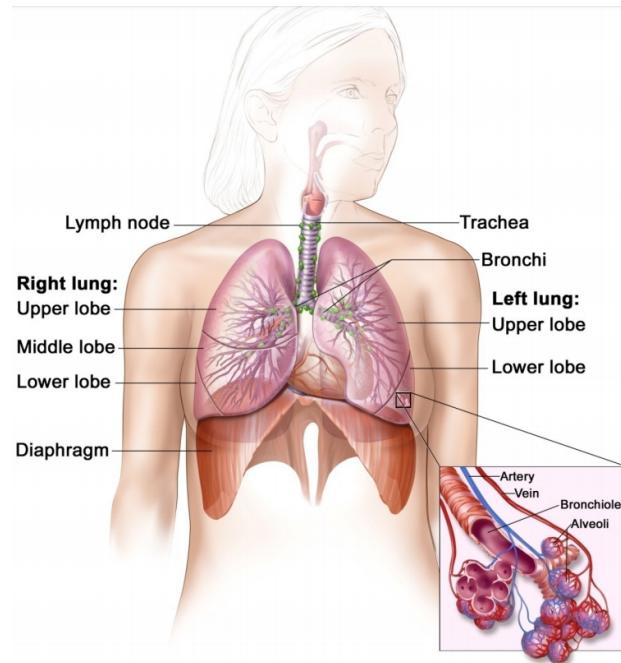


Figure 1.2: A medical drawing of the respiratory system [3].

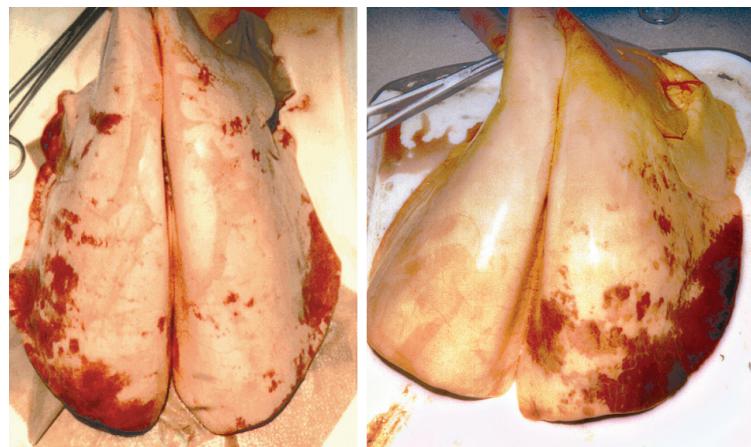


Figure 1.3: Lungs excised from animals (most likely ovine) who expired from injuries caused by a blast [4].

1.1. Problem Statement

Pulmonary contusion is one of the most common thoracic soft-tissue injuries caused by blunt trauma, with a mortality rate of 10-25% [5]. Damage to lungs is the main cause of morbidity following high-level blast exposures [6]. Lung laceration is also common and debilitating [7]. Existing constitutive models for lung tissue were developed from limited static test data, e.g., [8–10]. These models, and others developed since then, omit relevant physics pertinent to blast and ballistic impacts required to assess BABT. They also require cumbersome optimization protocols to fit non-unique parameter sets [11, 12], and/or are not validated against independent data [13]. Better lung models suitable for dynamic analysis are needed so that the Army can design improved PPE to better protect their soldiers.

The primary objective of the ARL-WMRD project *Modeling Large Deformations and Stress Wave Mechanics in Soft Biological Tissue* is to develop such models for deformation and damage/injury assessment. These are continuum models derived from thermodynamics that utilize internal state variables to account for the irreversible aspects of response [1, 2]. Models (both macroscopic and microscopic) are specifically sought whose parameters are physical and whose parameterization is straightforward. Characterization of the parameters in a model requires experimental data. This presents an enormous challenge, one that is being addressed in the ARL-WMRD project through other university collaborators.

Performing experiments for the purpose of model characterization is extremely difficult when it comes to modeling lung. Lung is a structure; parenchyma is a material. Therefore, one would normally choose to test the parenchyma, and from these data extract one's model parameters but, because of its spongy nature, we are challenged to do so in a physically meaningful way. Consequently, one typically tests whole lungs, or lobes thereof, and from these structural experiments we are tasked to extract material parameters through an inverse analysis. An alternative approach whereby one could, in principle, acquire parameters for the continuum models being developed at ARL-WMRD would be to homogenize a microscopic structural response for the alveoli of parenchyma. The work presented here addresses this approach in our modeling of deformation, damage and injury in alveolar structures.

The narrative that follows seeks to develop two material models for lung: one for mechanical deformation and the other for damage/injury/trauma. Models are sought whose parameters have physical interpretation. Ideally, they will enhance our understanding of the deformation and damage mechanisms at play during BABT. Specifically, they will describe how alveoli respond to pressure-waves and/or shear-waves as these wave fronts pass through them. This modeling will be accomplished by constructing a multi-scale model connecting the parenchyma (macro) and alveolar (micro) levels. In-silico experiments could then be done on the alveolar structural model, whose homogenized response could serve as an aid in the characterization of ARL's continuum models. The ARL-WMRD models are being designed to perform efficiently in their implementation in finite element codes. This will allow for BABT analyses to be done during the design of future PPE with an ultimate goal of saving soldiers' lives.

The primary purpose of this work is to provide a microscopic model for lung tissue that can be used as an aid in the parameterization of a macroscopic model for lung that will be

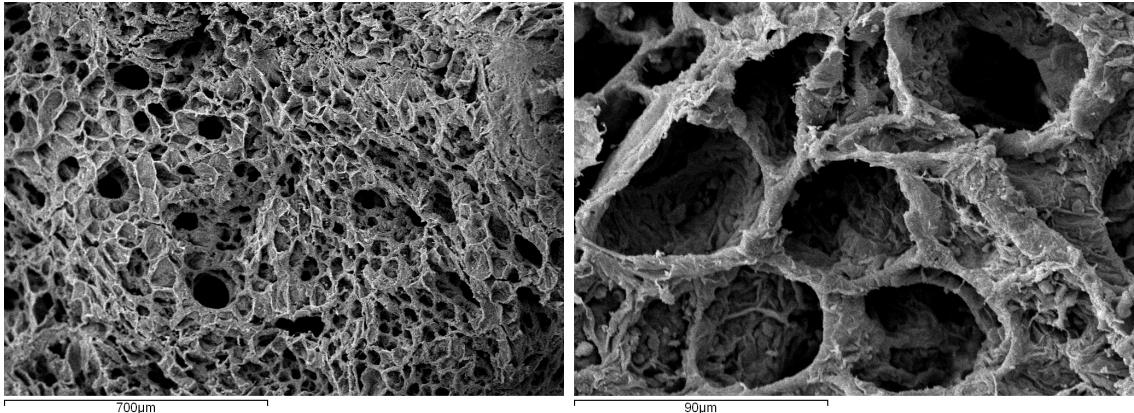


Figure 1.4: SEM photographs from a sectioned rat lung. Left image is at a magnification of 100X. Right image is at a magnification of 750X. They are Figs. 5 & 7 in Freed *et al.* [14]. The alveolar diameter in rat lung is about one quarter the alveolar diameter in human lung.

reasonably accurate yet efficient to run in full torso finite element analyses to study BABT.

1.2. Approach

Figure 1.4 shows micrographs from a rat lung taken at different magnifications [14]. In the lower-resolution image one sees numerous alveoli that became exposed because of the sectioning process. Also present are several alveolar ducts that connect the individual alveoli with the bronchial tree. In the higher-resolution image we observe the faceted structure of these alveoli, wherein one can see the septal chords and membranes, the latter being traversed by capillaries through which gas exchange occurs. Gas exchange will not modeled here.

Alveolar geometry is modeled here as a dodecahedron, i.e., a soccer-ball like structure comprised of twelve pentagonal facets bordered by thirty septal cords that are connected at twenty vertices. Each vertex links three neighboring cords of the alveolus with a fourth chord from a neighboring alveolus. BABT can occur through multiple mechanisms, e.g., tearing of septal cords and/or alveolar membranes, and in more severe cases, rupturing of capillaries can also happen causing blood to leak into neighboring alveoli, as seen in Fig. 1.5. Our dodecahedral model for alveoli is capable of capturing these trauma events.

Conjecture 1. *A microscopic strain field, measured at the scale of alveoli, is the same as its macroscopic strain field, measured at the scale of parenchyma. Deformation is affine.*

This hypothesis was tested and confirmed in an experimental study done by Butler *et al.* [16] where they used light scattering to study changes in geometry of the septal planes in alveoli from which they concluded: “the microscopic strain field does not differ significantly from the macroscopic field.” We employ this hypothesis by taking the deformation gradient from, say, a Gauss point in a finite element model of lung, e.g., from a Gauss point associated with Fig. 1.1, and imposing it as a far-field deformation onto our dodecahedral model of an alveolus. From this kinematic input we determine a macroscopic stress response homogenized from the microscopic forces created within this structural model for alveoli.

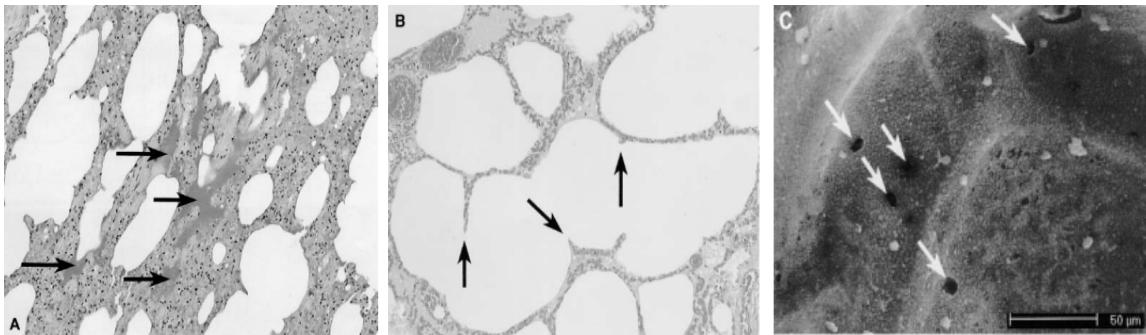


Figure 1.5: A) Immunohistochemical staining for hemoglobin showing edema fluid buildups (arrows) caused by blast injury. B) Histopathology image showing tearing of septal membranes (arrows) due to blast injury. C) Electron microscope image showing perforations (arrows) of the alveolar wall as a result of blast injury. All images are from Tsokos *et al.* [15].

The authors of a review article on alveolar strain finished by writing:

“In general, computational mechanics approaches to determine function in a healthy or diseased lung have proven to be useful in explaining or measuring observations that are not captured by imaging modalities. However, for these models to fully explain complex physiological mechanical events, appropriate mechanical properties, boundary conditions, and mechanical loads must be identified. Moreover, validation of such computational models, which is an essential component of any computational mechanics approach, remains to be a challenge in the analysis of soft tissue mechanics.”

Roan & Waters [17, pg. L633]

In this research we set out to develop a constitutive framework for alveolar mechanics, fully cognizant of the aforementioned challenges. Our objectives are different from those of prior studies in alveolar mechanics in that we seek to describe the response/injury of a human lung that has been subjected to a stress wave propagating across the thorax region caused by an impact from either a blunt object or a blast wave. Consequently, some important aspects in the modeling of a breathing lung are thought to be less impactful here, e.g., the effect of surfactant in keeping alveoli from collapsing at the end of expiration.

As a foundation, we adopt the guideline:

“Constitutive equations are phenomenological. They are regarded as empirical by experimenters, and axiomatic by mathematicians. In biomechanics, we often try to derive them on the basis of microstructure . . . in order to gain a better understanding, or to get some guidance to the mathematical form.”

Y.-C. Fung [18, pg. 431]

The approach adopted here is to use the geometry of a dodecahedron as a *microscopic* mechanical model for alveoli, whose far-field response to mechanical stimuli, in accordance with Conjecture 1, will be used to inform the development of a *macroscopic* mechanical model for parenchyma [1], the predominant tissue in lung. This is deemed necessary because of the complex porous structure of parenchyma, as compared with the homogeneous structure of

rubbery elastic solids whose theories have historically been employed to model parenchyma [8, 9, 19, 20]. The ARL-WMRD continuum (macroscopic) model for parenchyma [1] will be implemented into finite element codes by others on our team with an end objective being improved and more effective designs for protective body armor.

1.3. Organization

This document is organized in the following manner. Part 2 introduces the dodecahedron as a model for alveoli. Its geometric properties are derived in detail with regards to its three geometric features: 1D septal chords, 2D septal membranes, and 3D volume. Part 3 develops the kinematics required for us to model a deforming dodecahedron, again focusing on the 1D chords, 2D membranes, and the 3D volume within. Part 4 derives constitutive models suitable for describing the thermo-mechanical response for the structural constituents of an alveolus: its septal chords, its permeable membranes, and its volume. Part 5 presents numerical methods used for solving first-order parabolic and second-order hyperbolic, ordinary, differential equations (ODEs), and for solving spatial integrations along a bar, across a pentagon, and throughout a tetrahedron using Gaussian quadrature schemes designed for each geometry. Part 6 describes a variational formulation used to create our structural model of an alveolus, which consists of three models: one comprised of septal chords, another comprised of septal membranes, and the third comprised of alveolar volume. All interpolate their stresses to the vertices where the forces from each are summed and homogenized for return to the macroscopic solver. The first appendix provides an overview of implicit constitutive equations used in our alveolar model. The remaining appendices provide a reference manual for the software developed to accomplish this project's objective, which was written in Python vs. 3.7.

Part 2

Dodecahedra: A Model for Alveoli

Typical alveoli are fourteen sided polyhedra with one face normally being open as a mouth to an alveolar duct, and whose septal membranes typically become flat at transpulmonary pressures as low as 2 cm H₂O [21]. To capture the microstructural features of lung, researchers have modeled both alveoli and alveolar ducts, as seen in Fig. 1.4; we only address alveoli here. Three different geometric shapes are typically employed when modeling an alveolus: a dodecahedron introduced by Frankus & Lee [22] in 1974, a rhombic dodecahedron introduced by de Ryk, Thiesse, Namati & McLennan [23] in 2007, and a truncated octahedron, i.e., a tetrakaidecahedron, introduced by Dale, Matthews & Schroter [24] in 1980. The dodecahedron and rhombic dodecahedron are both twelve sided polyhedra with faces being pentagons and rhombuses, respectively. A tetrakaidecahedron is a pair of pyramids stacked bottom to bottom, forming an octahedron, whose six points are then removed. The end result is a fourteen sided polyhedron with six faces that are squares and eight faces that are hexagons, where like shapes have like dimensions.

The tetrakaidecahedron and rhombic dodecahedron are both volume filling. This property is preferred whenever one sets out to construct assemblages of alveoli to build a microstructural model that is to be solved numerically via a finite element method. The purpose of such an exercise is to homogenize the response of an alveolar assembly up to the macroscopic level, i.e., the level of a continuum mass point, a.k.a., the parenchyma [23–29]. Such a finite element model can serve as a representative volume element (RVE) for parenchyma.

The dodecahedron is an isotropic structure, or very nearly so as we shall show, and is nearly volume filling [30]. It becomes a preferred geometry whenever a single alveolus is to be used as the RVE of homogenization, and from which closed form solutions have been derived [14, 30–32]. Here isotropy of the microstructure ensures an isotropic macro response. Parenchyma, as a tissue, is isotropic [20, 33, 34]; whereas, lung, as an organ, is a complex, heterogeneous structure [35, 36]. This distinction has, from time-to-time, gotten lost [37].

For the reasons stated above, a dodecahedron, with vertices labeled according to Fig. 2.1, is the geometric structure selected for use in this study. The question of how one assigns a co-ordinate system to a dodecahedron is discussed first. Given this co-ordinate system, vertices of a dodecahedron are then assigned from which its septal chords and septal membranes are established.

2.1. Co-ordinate Indexing

An orthonormal set of base vectors $(\vec{i}, \vec{j}, \vec{k})$ is assigned to a dodecahedron whose origin resides at its centroid and whose directions align with a set of far-field base vectors used for reference in one's finite element model of a lung. The question is: How does one orient the indexing scheme of Fig. 2.1 against this basis? Alternatively: How can one describe a mapping $(\vec{i}, \vec{j}, \vec{k}) \xrightarrow{?} (\vec{E}_1, \vec{E}_2, \vec{E}_3)$ wherein the orthonormal set of base vectors $(\vec{E}_1, \vec{E}_2, \vec{E}_3)$ is

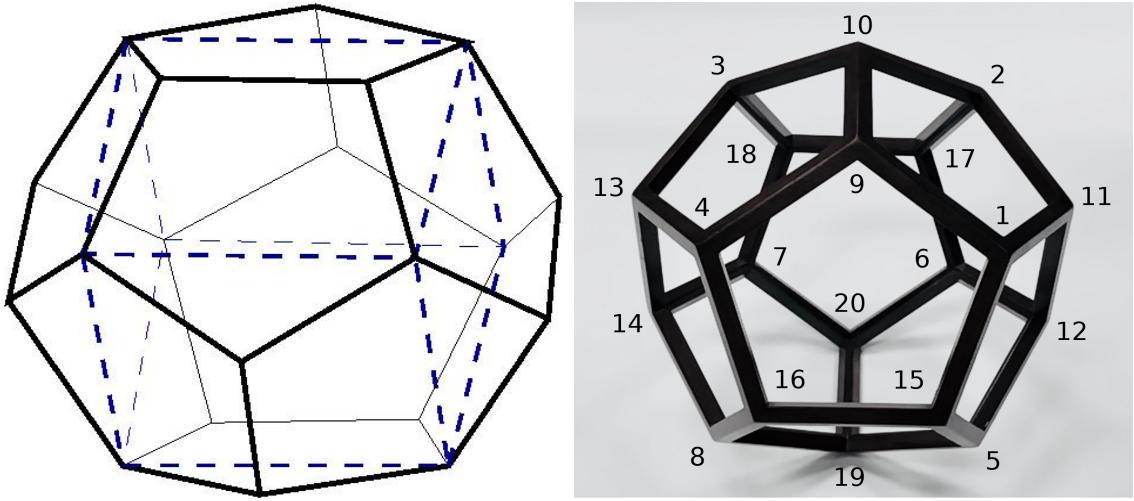


Figure 2.1: Geometric representations for a dodecahedron. Left image: A cube is contained within a dodecahedron, with one of its five possible orientations being displayed. Atop each face of the cube resides four pentagonal sub-areas that form the shape of a hipped roof line. Right image: Vertices 1 through 8 are located at the corners of such a cube. The centroid for the cube is also the centroid for the dodecahedron. Vertices 9 through 20 are corners of the hipped roof lines residing above each face of the cube.

to serve as a reference basis for our alveolar dodecahedron to which the indexing scheme presented in Fig. 2.1 applies?

Given that a finite element model for lung exists, then a deformation gradient \mathbf{F} can be made available at any mass point therein whereat an alveolus of interest resides. The components of this deformation gradient are F_{ij} , $i, j = 1, 2, 3$, when evaluated in the co-ordinate frame $(\vec{i}, \vec{j}, \vec{k})$, which is the co-ordinate frame of the finite element analysis. A Gram-Schmidt (or QR) decomposition of a non-singular 3×3 matrix results in a tangent vector \vec{g}_1 and normal vector $\vec{g}_1 \times \vec{g}_2$ that remain invariant under transformations of the triangular matrix \mathbf{R} [38]. These convected base vectors $(\vec{g}_1, \vec{g}_2, \vec{g}_3)$ rotate out of basis $(\vec{E}_1, \vec{E}_2, \vec{E}_3)$ via a Gram rotation [39]. Given this geometric information, Paul, Rajagopal & Freed [40] were able to provide an answer to the above question of co-ordinate selection.

Their approach begins by establishing the extent of transverse shear crossing each of the co-ordinate directions $(\vec{i}, \vec{j}, \vec{k})$, as quantified by

$$\mathcal{G}_1 = \frac{\sqrt{F_{21}^2 + F_{31}^2}}{F_{11}}, \quad \mathcal{G}_2 = \frac{\sqrt{F_{12}^2 + F_{32}^2}}{F_{22}}, \quad \mathcal{G}_3 = \frac{\sqrt{F_{13}^2 + F_{23}^2}}{F_{33}} \quad (2.1)$$

where \mathcal{G}_i is a measure of the shear deformation cutting across the i^{th} direction. Unit vector \vec{E}_1 is selected as that direction from the set $\{\vec{i}, \vec{j}, \vec{k}\}$ which possesses minimal transverse shear. Once selected, there are two possible planes that contain base vector \vec{E}_1 , and the one selected whose normal is to be $\vec{E}_1 \times \vec{E}_2$ is that plane with the least amount of in-plane shear, as determined by taking appropriate dot products between column vectors $\mathbf{f}_i = \{F_{1i} \ F_{2i} \ F_{3i}\}^T$, $i = 1, 2, 3$. Vector \mathbf{f}_i has elements taken from the i^{th} column of matrix F_{ij} , which represents the deformation gradient \mathbf{F} evaluated in $(\vec{i}, \vec{j}, \vec{k})$. Their strategy is summarized in Alg. 1.

Algorithm 1 inputs a deformation gradient \mathbf{F} whose components F_{ij} are evaluated in the co-ordinate system $(\vec{i}, \vec{j}, \vec{k})$ associated with a finite element model for lung. The algorithm outputs an orthogonal matrix \mathbf{P} that re-indexes the components of the deformation gradient F_{ij} into an equivalent form where $\mathbf{F} = \mathcal{F}_{ij} \vec{\mathbf{E}}_i \otimes \vec{\mathbf{E}}_j$. It is this re-indexed matrix \mathcal{F}_{ij} that is to be subjected to Gram-Schmidt factorization later in Part 3.

Algorithm 1: Pivoting of the co-ordinate system.

Input: Deformation gradient \mathbf{F} with components F_{ij} expressed in $(\vec{i}, \vec{j}, \vec{k})$.

if $\mathcal{G}_1 \leq \mathcal{G}_2$ and $\mathcal{G}_1 \leq \mathcal{G}_3$ **then**

- if** $f_1 \cdot f_2 \leq f_1 \cdot f_3$ **then**

 - $[\mathcal{F}_1] = [\mathbf{P}_1]^T [\mathbf{F}] [\mathbf{P}_1]$, $[\mathcal{F}] = [\mathcal{F}_1]$, $[\mathbf{P}] = [\mathbf{P}_1]$, $\therefore (\vec{i}, \vec{j}, \vec{k}) \mapsto (\vec{\mathbf{E}}_1, \vec{\mathbf{E}}_2, \vec{\mathbf{E}}_3)$

- else**

 - $[\mathcal{F}_2] = [\mathbf{P}_2]^T [\mathbf{F}] [\mathbf{P}_2]$, $[\mathcal{F}] = [\mathcal{F}_2]$, $[\mathbf{P}] = [\mathbf{P}_2]$, $\therefore (\vec{i}, \vec{j}, \vec{k}) \mapsto (\vec{\mathbf{E}}_1, \vec{\mathbf{E}}_3, \vec{\mathbf{E}}_2)$

else if $\mathcal{G}_2 \leq \mathcal{G}_1$ and $\mathcal{G}_2 \leq \mathcal{G}_3$ **then**

- if** $f_1 \cdot f_2 \leq f_2 \cdot f_3$ **then**

 - $[\mathcal{F}_3] = [\mathbf{P}_3]^T [\mathbf{F}] [\mathbf{P}_3]$, $[\mathcal{F}] = [\mathcal{F}_3]$, $[\mathbf{P}] = [\mathbf{P}_3]$, $\therefore (\vec{i}, \vec{j}, \vec{k}) \mapsto (\vec{\mathbf{E}}_2, \vec{\mathbf{E}}_1, \vec{\mathbf{E}}_3)$

- else**

 - $[\mathcal{F}_4] = [\mathbf{P}_4]^T [\mathbf{F}] [\mathbf{P}_4]$, $[\mathcal{F}] = [\mathcal{F}_4]$, $[\mathbf{P}] = [\mathbf{P}_4]$, $\therefore (\vec{i}, \vec{j}, \vec{k}) \mapsto (\vec{\mathbf{E}}_2, \vec{\mathbf{E}}_3, \vec{\mathbf{E}}_1)$

else

- if** $f_1 \cdot f_3 \leq f_2 \cdot f_3$ **then**

 - $[\mathcal{F}_5] = [\mathbf{P}_5]^T [\mathbf{F}] [\mathbf{P}_5]$, $[\mathcal{F}] = [\mathcal{F}_5]$, $[\mathbf{P}] = [\mathbf{P}_5]$, $\therefore (\vec{i}, \vec{j}, \vec{k}) \mapsto (\vec{\mathbf{E}}_3, \vec{\mathbf{E}}_1, \vec{\mathbf{E}}_2)$

- else**

 - $[\mathcal{F}_6] = [\mathbf{P}_6]^T [\mathbf{F}] [\mathbf{P}_6]$, $[\mathcal{F}] = [\mathcal{F}_6]$, $[\mathbf{P}] = [\mathbf{P}_6]$, $\therefore (\vec{i}, \vec{j}, \vec{k}) \mapsto (\vec{\mathbf{E}}_3, \vec{\mathbf{E}}_2, \vec{\mathbf{E}}_1)$

Output: Deformation gradient \mathbf{F} with components \mathcal{F}_{ij} expressed in $(\vec{\mathbf{E}}_1, \vec{\mathbf{E}}_2, \vec{\mathbf{E}}_3)$ as re-indexed by an orthogonal matrix $[\mathbf{P}]$.

There are six cases that can arise. Their associated orthogonal matrices are

$$\begin{aligned} [\mathbf{P}_1] &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} & [\mathbf{P}_2] &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} & [\mathbf{P}_3] &= \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \\ [\mathbf{P}_4] &= \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} & [\mathbf{P}_5] &= \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} & [\mathbf{P}_6] &= \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \end{aligned} \quad (2.2a)$$

whose affiliated components for the re-indexed deformation gradient are

$$\begin{aligned} [\mathcal{F}_1] &= \begin{bmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{bmatrix} & [\mathcal{F}_2] &= \begin{bmatrix} F_{11} & F_{13} & F_{12} \\ F_{31} & F_{33} & F_{32} \\ F_{21} & F_{23} & F_{22} \end{bmatrix} & [\mathcal{F}_3] &= \begin{bmatrix} F_{22} & F_{21} & F_{23} \\ F_{12} & F_{11} & F_{13} \\ F_{32} & F_{31} & F_{33} \end{bmatrix} \\ [\mathcal{F}_4] &= \begin{bmatrix} F_{22} & F_{23} & F_{21} \\ F_{32} & F_{33} & F_{31} \\ F_{12} & F_{13} & F_{11} \end{bmatrix} & [\mathcal{F}_5] &= \begin{bmatrix} F_{33} & F_{31} & F_{32} \\ F_{13} & F_{11} & F_{12} \\ F_{23} & F_{21} & F_{22} \end{bmatrix} & [\mathcal{F}_6] &= \begin{bmatrix} F_{33} & F_{32} & F_{31} \\ F_{23} & F_{22} & F_{21} \\ F_{13} & F_{12} & F_{11} \end{bmatrix} \end{aligned} \quad (2.2b)$$

where case 1 is the default case whose operator \mathbf{P}_1 is the identity tensor.

All vectors \mathbf{V} with components \mathcal{V}_i evaluated in $(\vec{\mathbf{E}}_1, \vec{\mathbf{E}}_2, \vec{\mathbf{E}}_3)$ will rotate into $(\vec{\mathbf{i}}, \vec{\mathbf{j}}, \vec{\mathbf{k}})$ with components V_i according to the map

$$V_i = P_{ij}\mathcal{V}_j \quad \text{or inversely} \quad \mathcal{V}_i = P_{ji}V_j \quad (2.3a)$$

while all tensors \mathbf{T} with components \mathcal{T}_{ij} evaluated in $(\vec{\mathbf{E}}_1, \vec{\mathbf{E}}_2, \vec{\mathbf{E}}_3)$ will rotate into $(\vec{\mathbf{i}}, \vec{\mathbf{j}}, \vec{\mathbf{k}})$ with components T_{ij} according to the map

$$T_{ij} = P_{ik}\mathcal{T}_{kl}P_{lj} \quad \text{or inversely} \quad \mathcal{T}_{ij} = P_{ki}T_{kl}P_{lj} \quad (2.3b)$$

where the latter appears in Alg. 1 with regards to components of the deformation gradient.

From this point onward, it is assumed that base vectors $(\vec{\mathbf{E}}_1, \vec{\mathbf{E}}_2, \vec{\mathbf{E}}_3)$ are known, and that they serve as the reference basis for our alveolar analysis.

2.2. Geometric Properties of a Regular Pentagon

Figure 2.2 presents a regular pentagon drawn in its natural co-ordinate system with coordinates designated as (ξ, η) . Vertices of such a pentagon are placed at

$$\xi = \cos\left(\frac{2(k-1)\pi}{5} + \frac{\pi}{2}\right) \quad \eta = \sin\left(\frac{2(k-1)\pi}{5} + \frac{\pi}{2}\right) \quad k = 1, 2, \dots, 5 \quad (2.4)$$

wherein k denotes the vertex number, as assigned in Fig. 2.2. These vertices inscribe a pentagon within the unit circle.

Lengths of the five chords in a regular pentagon, when measured in its natural co-ordinate system, are all

$$L^p = 2\cos(\omega) \approx 1.176 \quad (2.5)$$

while the area of this pentagon is

$$A^p = \frac{5}{4}\tan(\omega)L^p{}^2 = 5\sin(\omega)\cos(\omega) \approx 2.378 \quad (2.6)$$

where the area of an unit circle is $\pi r^2 \approx 3.142$ because $r = 1$. The inside angles of a regular pentagon all measure $2\omega = 108^\circ$. All approximations are truncated at four significant figures.

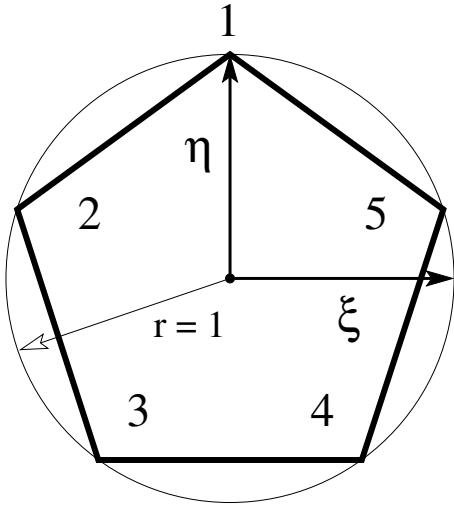


Figure 2.2: A regular pentagon inscribed within the unit circle establishes its natural coordinate system with co-ordinates (ξ, η) described in Eqn. (2.4), and whose origin is located at its centroid. Vertices are numbered counterclockwise with the uppermost vertex being labeled 1.

2.3. Geometric Properties of a Regular Dodecahedron

Like the pentagon considered above, which inscribes the unit circle, here we consider a dodecahedron that inscribes the unit sphere. Let this geometry be described in its natural co-ordinate system with co-ordinates (ξ, η, ζ) whose origin is located at its centroid, the center of the sphere. The twenty vertices of this dodecahedron, all of which touch the unit sphere, are placed at

$$\begin{array}{ccc} \xi & \eta & \zeta \\ \hline \pm 1/\sqrt{3} & \pm 1/\sqrt{3} & \pm 1/\sqrt{3} \\ \pm \phi/\sqrt{3} & \pm 1/\sqrt{3}\phi & 0 \\ 0 & \pm \phi/\sqrt{3} & \pm 1/\sqrt{3}\phi \\ \pm 1/\sqrt{3}\phi & 0 & \pm \phi/\sqrt{3} \end{array} \quad (2.7)$$

where $\phi = (1 + \sqrt{5})/2 \approx 1.618$ is also known as the golden ratio.

Lengths of the thirty chords in a regular dodecahedron, when measured in its natural co-ordinate system, are all

$$L^d = \frac{2}{\sqrt{3}\phi} \approx 0.7136 \quad (2.8)$$

while the volume of such a dodecahedron is

$$V^d = \frac{40}{3\sqrt{3}\phi^3} \tan^2(\omega) \sin(\omega) \approx 2.785 \quad (2.9)$$

where volume of the unit sphere is $\frac{4}{3}\pi r^3 \approx 4.189$ because $r = 1$.

The scale factor to map between the natural co-ordinates of a pentagon, defined in Eq. (2.4), with those of a dodecahedron, defined in Eq. (2.7), is

$$\frac{L^p}{R^p} = \frac{L^d}{R_d^p} \quad \text{or} \quad R_d^p = \frac{R^p L^d}{L^p} = \frac{L^d}{L^p} = \frac{1}{\sqrt{3}\phi \cos(\omega)} \approx 0.6071 \quad (2.10)$$

because $R^p = 1$, with scale factor R_d^p being the radius that inscribes a pentagon on the surface of a dodecaheron that itself inscribes the unit sphere.

2.4. Dimensions of Human Alveoli

Septal chord length $L(D)$, expressed as a function of alveolar diameter D , can be estimated by considering the areal projection of a dodecahedron onto a plane that contains one of its pentagonal faces, which leads to

$$L = \frac{D}{\tan(\omega)(1 + \cos(\alpha))} \approx \frac{D}{2.685}, \quad (2.11)$$

where $\alpha = \pi/10 = 18^\circ$. (There are twenty, equal, pie-shaped wedges that comprise this projected area.) This is an average of the shortest and longest distances across this plane of projection. Alveolar diameter D is a property that can be measured during an histological study of parenchyma.

To dimension the alveoli of human lung, Sabin, Fung & Tremer [41] measured the mean diameter across an individual alveolus, viz., D of Eq. (2.11), sectioned from human lungs that were fixed at three different pressures. Samples were taken from nine lungs extracted postmortem from individuals between 16 to 89 years of age.¹ At a transpulmonary pressure of 4 cm H₂O, the mean alveolar diameter was $D = 191 \pm 86 \mu\text{m}$ determined from a sampling size of 1423; at a pressure of 10 cm H₂O, $D = 202 \pm 88 \mu\text{m}$ determined from a sampling size of 1296; and at a pressure of 14 cm H₂O, $D = 235 \pm 99 \mu\text{m}$ determined from a sampling size of 1083. These data are plotted in Fig. 2.3. All reported and drawn error bounds pertain to plus/minus one standard deviation in error.

2.5. Geometric Properties for Irregular Pentagons and Dodecahedra

Formulæ (2.6 & 2.9) only apply for regular pentagons and dodecahedra evaluated in their respective natural co-ordinate systems. For irregular dodecahedra, the areas of its irregular pentagons are calculated via²

$$A = \frac{1}{2} \sum_{i=1}^5 (x_i y_{i+1} - x_{i+1} y_i) \quad (2.12)$$

¹Sabin *et al.* [41] documented an age effect in these data that has been averaged over here, i.e., ignored.

²Bourke, P., “Polygons, Meshes.” <http://paulbourke.net/geometry>.

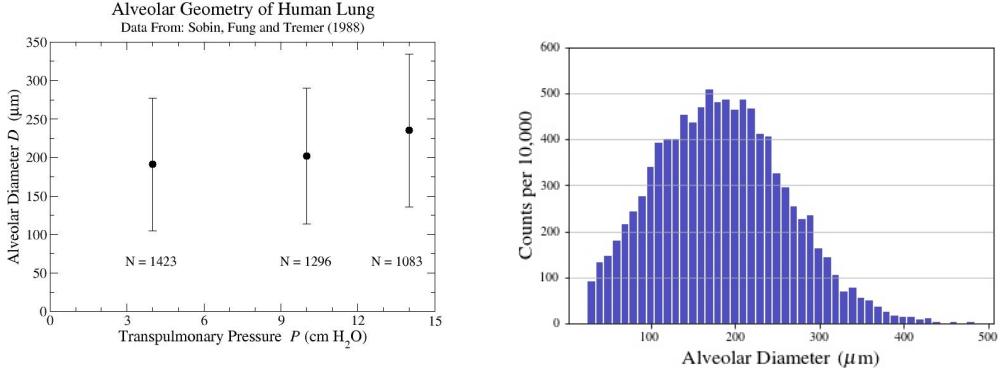


Figure 2.3: Mean and standard deviations for alveolar diameter in human lung illustrated in the left graphic, as reported by Sabin *et al.* [41], with a typical histogram for these statistics illustrated in the right graphic. Note that this distribution has been truncated at an alveolar diameter of 24 μm .

where $x_6 \Leftarrow x_1$ and $y_6 \Leftarrow y_1$. In order for the predicted area to be positive when using this formula, it is necessary that the vertices (x_i, y_i) index counterclockwise, as drawn in Fig. 2.2. The centroid of this pentagon has co-ordinates²

$$c_x = \frac{1}{6A} \sum_{i=1}^5 (x_i + x_{i+1})(x_i y_{i+1} - x_{i+1} y_i) \quad (2.13a)$$

$$c_y = \frac{1}{6A} \sum_{i=1}^5 (y_i + y_{i+1})(x_i y_{i+1} - x_{i+1} y_i) \quad (2.13b)$$

wherein the vertex co-ordinates x_i and y_i are quantified in a 2D pentagonal frame of reference, e.g., as established later in Fig. 2.5.

To compute the volume of an irregular dodecahedron, use the formula³

$$288 V_{tet}^2 = \begin{vmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & \ell_{12}^2 & \ell_{13}^2 & \ell_{14}^2 \\ 1 & \ell_{21}^2 & 0 & \ell_{23}^2 & \ell_{24}^2 \\ 1 & \ell_{31}^2 & \ell_{32}^2 & 0 & \ell_{34}^2 \\ 1 & \ell_{41}^2 & \ell_{42}^2 & \ell_{43}^2 & 0 \end{vmatrix} \quad (2.14)$$

to calculate each of the 60 individual tetrahedral volumes that collectively fill the volume of an irregular dodecahedron. Here ℓ_{ij} is the length of that tetrahedral edge with vertices i and j ; $i, j = 1, 2, 3, 4$; $i \neq j$; with $\ell_{ij} = \ell_{ji}$.

2.6. Indexing Scheme for Dodecahedra

In order to implement the dodecahedron as a geometric model for an alveolar sac, as suggested by the images in Fig. 1.4, it first becomes necessary to introduce a labeling strategy.

³Colins, K. D., “Cayley-Menger Determinant.” From MathWorld—A Wolfram Web Resource, created by Eric W. Weisstein. <http://mathworld.wolfram.com/CayleyMengerDeterminant.html>.

Vertex	ξ	η	ζ	Vertex	ξ	η	ζ
1	$1/\sqrt{3}$	$1/\sqrt{3}$	$1/\sqrt{3}$	11	$\phi/\sqrt{3}$	$1/\sqrt{3}\phi$	0
2	$1/\sqrt{3}$	$1/\sqrt{3}$	$-1/\sqrt{3}$	12	$\phi/\sqrt{3}$	$-1/\sqrt{3}\phi$	0
3	$-1/\sqrt{3}$	$1/\sqrt{3}$	$-1/\sqrt{3}$	13	$-\phi/\sqrt{3}$	$1/\sqrt{3}\phi$	0
4	$-1/\sqrt{3}$	$1/\sqrt{3}$	$1/\sqrt{3}$	14	$-\phi/\sqrt{3}$	$-1/\sqrt{3}\phi$	0
5	$1/\sqrt{3}$	$-1/\sqrt{3}$	$1/\sqrt{3}$	15	$1/\sqrt{3}\phi$	0	$\phi/\sqrt{3}$
6	$1/\sqrt{3}$	$-1/\sqrt{3}$	$-1/\sqrt{3}$	16	$-1/\sqrt{3}\phi$	0	$\phi/\sqrt{3}$
7	$-1/\sqrt{3}$	$-1/\sqrt{3}$	$-1/\sqrt{3}$	17	$1/\sqrt{3}\phi$	0	$-\phi/\sqrt{3}$
8	$-1/\sqrt{3}$	$-1/\sqrt{3}$	$1/\sqrt{3}$	18	$-1/\sqrt{3}\phi$	0	$-\phi/\sqrt{3}$
9	0	$\phi/\sqrt{3}$	$1/\sqrt{3}\phi$	19	0	$-\phi/\sqrt{3}$	$1/\sqrt{3}\phi$
10	0	$\phi/\sqrt{3}$	$-1/\sqrt{3}\phi$	20	0	$-\phi/\sqrt{3}$	$-1/\sqrt{3}\phi$

Table 2.1: Natural co-ordinates for the vertices of a regular dodecahedron, as labeled in Fig. 2.1 according to Eq. (2.7).

Such a scheme is arbitrary, but once chosen it enables an analysis to be put forward. The labeling scheme adopted in this work is illustrated in the right image of Fig. 2.1.

The co-ordinates positioning the twenty vertices of a regular dodecahedron in its natural frame of reference are presented in Table 2.1. According to the labeling scheme of Fig. 2.1, the thirty chords of a dodecahedron are given vertex assignments according to Table 2.2, while its twelve pentagons are given vertex assignments according to Table 2.3.

The sixty tetrahedra that fill the volume of the dodecahedron contain vertices according to the following strategy. Beginning with pentagon 1 and sequencing to pentagon 12, two of the four vertices come from a side of the pentagon in question with the remaining two vertices being the centroid for the associated pentagon and the centroid for the dodecahedron, i.e., the co-ordinate origin. From Table 2.3, tetrahedron 1 contains vertices 11 and 2 of pentagon 1, tetrahedron 2 contains vertices 2 and 10, tetrahedron 3 contains vertices 10 and 9, tetrahedron 4 contains vertices 9 and 1, tetrahedron 5 contains vertices 1 and 11, tetrahedron 6 contains vertices 10 and 2 from pentagon 2, etc.

2.7. Co-ordinate Systems for Chordal Fibers and Pentagonal Membranes

The dodecahedron used to model an alveolus is considered to be regular in its ‘natural’ configuration, with the capability of being irregular in its reference configuration, and certainly becoming irregular after deformation. The co-ordinate frame of its natural state is taken to have its origin positioned at the centroid of this regular dodecahedron, i.e., at the centroid of its enclosed cube (cf. Fig. 2.1) or, equivalently, at the origin of that unit sphere for which the dodecahedron inscribes, as presented in Table 2.1. We denote the base vectors associated with this frame of reference as $(\vec{\mathbf{E}}_1, \vec{\mathbf{E}}_2, \vec{\mathbf{E}}_3)$, assigned according to §2.1. There are two other co-ordinate systems with relevance to our analysis: those for the chordal fibers, and those for the pentagonal membranes.

Chord	Vertices	Chord	Vertices	Chord	Vertices
1	9, 10	11	17, 18	21	7, 18
2	1, 9	12	3, 18	22	7, 14
3	2, 10	13	4, 16	23	13, 14
4	3, 10	14	15, 16	24	8, 14
5	4, 9	15	1, 15	25	8, 16
6	1, 11	16	5, 15	26	5, 19
7	2, 11	17	5, 12	27	6, 20
8	3, 13	18	11, 12	28	7, 20
9	4, 13	19	6, 12	29	8, 19
10	2, 17	20	6, 17	30	19, 20

Table 2.2: Vertices that locate the endpoints of septal chords in a dodecahedron, as labeled in Fig. 2.1.

Pentagon	Vertices	Chords
1	11, 2, 10, 9, 1	6, 7, 3, 1, 2
2	10, 2, 17, 18, 3	4, 3, 10, 11, 12
3	13, 4, 9, 10, 3	8, 9, 5, 1, 4
4	9, 4, 16, 15, 1	2, 5, 13, 14, 15
5	15, 5, 12, 11, 1	15, 16, 17, 18, 6
6	17, 2, 11, 12, 6	20, 10, 7, 18, 19
7	18, 7, 14, 13, 3	12, 21, 22, 23, 8
8	16, 4, 13, 14, 8	25, 13, 9, 23, 24
9	12, 5, 19, 20, 6	19, 17, 26, 30, 27
10	14, 7, 20, 19, 8	24, 22, 28, 30, 29
11	20, 7, 18, 17, 6	27, 28, 21, 11, 20
12	19, 5, 15, 16, 8	29, 26, 16, 14, 25

Table 2.3: Vertices that locate the corners of regular pentagonal surfaces in a regular dodecahedron, and the chords that connect them. They are indexed counterclockwise when viewed looking from the outside in, and labeled according to Fig. 2.1. The apex for each pentagon resides at the peak of the hipped roof-line for that pentagon. This turns out to be important.

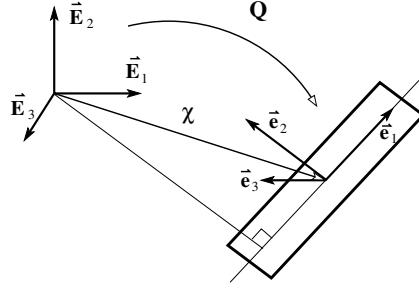


Figure 2.4: The co-ordinate system of a chord ($\vec{e}_1, \vec{e}_2, \vec{e}_3$) relative to the co-ordinate system of its dodecahedron ($\vec{\mathbf{E}}_1, \vec{\mathbf{E}}_2, \vec{\mathbf{E}}_3$) with origins located at their respective centroids that are offset by a translation χ . These describe a mapping $[\{\vec{e}_1\}\{\vec{e}_2\}\{\vec{e}_3\}] = [\{\vec{\mathbf{E}}_1\}\{\vec{\mathbf{E}}_2\}\{\vec{\mathbf{E}}_3\}][\mathbf{Q}]$ where \mathbf{Q} is an orthogonal rotation. The tangent base vector \vec{e}_1 aligns with the axis of this chord. The normal base vector \vec{e}_2 is coaxial with a line segment drawn from the origin out to the chordal axis such that $\vec{e}_1 \cdot \vec{e}_2 = 0$. While the binormal base vector is given by the cross product $\vec{e}_3 = \vec{e}_1 \times \vec{e}_2$.

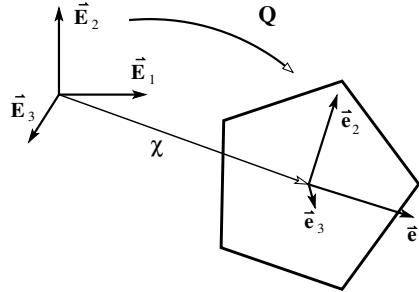


Figure 2.5: The co-ordinate system of a pentagon ($\vec{e}_1, \vec{e}_2, \vec{e}_3$) relative to the co-ordinate system of its dodecahedron ($\vec{\mathbf{E}}_1, \vec{\mathbf{E}}_2, \vec{\mathbf{E}}_3$) with origins located at their respective centroids that are offset by a translation χ . These describe a mapping $[\{\vec{e}_1\}\{\vec{e}_2\}\{\vec{e}_3\}] = [\{\vec{\mathbf{E}}_1\}\{\vec{\mathbf{E}}_2\}\{\vec{\mathbf{E}}_3\}][\mathbf{Q}]$ where \mathbf{Q} is an orthogonal rotation. Base vector \vec{e}_1 is coaxial to a line segment that connects two vertices which locate a pair of shoulders in a pentagon, viz., vertices 2 and 5 in Fig. 2.2. Base vector \vec{e}_2 is coaxial with a line segment drawn from the head of this pentagon, i.e., vertex 1 in Fig. 2.2, down to its base such that $\vec{e}_1 \cdot \vec{e}_2 = 0$. Base vector $\vec{e}_3 = \vec{e}_1 \times \vec{e}_2$ is the outward normal to this surface.

The local co-ordinate system of a chordal fiber is presented in Fig. 2.4, while the local co-ordinate system of a pentagonal membrane is presented in Fig. 2.5. The software described in Appendix E and Appendix F utilize these co-ordinate systems, whose origins are located at their centroids, along with their rotation and spin matrices, which are measured relative to the co-ordinate frame of the dodecahedron, i.e., relative to $(\vec{\mathbf{E}}_1, \vec{\mathbf{E}}_2, \vec{\mathbf{E}}_3)$.

Part 3

Kinematics

The irregular dodecahedron used here as a model for alveoli describes a 3D structure composed of thirty 1D rods (the septal chords) joined at twenty nodes (the vertices) that collectively circumscribe twelve 2D pentagonal membranes (the alveolar septa) that in turn envelop an alveolar sac whose volume is represented using sixty tetrahedra. To be able to describe the overall mechanical response of this 3D dodecahedral structure, it is conjectured to be sufficient to know the individual mechanical responses of its 1D septal chords, its 2D septal membranes, and the 3D void within. Their relevant kinematics are presented here, along with the shape functions used for interpolation and our description of deformation.

3.1. 1D Chords

The stretch of a rod under extension is a ratio of its lengths. Specifically, $\lambda := L/L_0$ where L and L_0 are its current and reference lengths, respectively, whose strain and strain rate are taken to be $e = \ln \lambda$ and $de = \lambda^{-1}d\lambda$. This is often referred to as a logarithmic, natural or true strain. Consequently, the kinematic analysis of a chord is trivial.

3.1.1. Shape Functions for Interpolating a Rod

A two-noded alveolar chord has shape functions N_i , $i = 1, 2$, that, when evaluated in its natural coordinate system where $-1 \leq \xi \leq 1$, describe a matrix with elements

$$\mathbf{N} = [N_1 \ N_2] = \left[\frac{1}{2}(1 - \xi) \quad \frac{1}{2}(1 + \xi) \right] \quad (3.1a)$$

that interpolate vector fields according to

$$\mathbf{x}(\xi) = \sum_{i=1}^2 N_i(\xi) x_i, \quad \mathbf{u}(\xi) = \sum_{i=1}^2 N_i(\xi) u_i \quad (3.1b)$$

etc., and whose spatial gradients are

$$N_{1,\xi} = -\frac{1}{2} \quad \text{and} \quad N_{2,\xi} = \frac{1}{2} \quad (3.1c)$$

wherein ξ is the natural co-ordinate. Components x_i and $u_i := x_i - x_{0i}$ are their global co-ordinates and displacements, respectively, located at the two nodes of a chord evaluated in the co-ordinate frame $(\vec{\mathbf{e}}_1, \vec{\mathbf{e}}_2, \vec{\mathbf{e}}_3)$ of Fig. 2.4 with the chordal axis lying in the $\vec{\mathbf{e}}_1$ direction.

3.1.2. Deformation Gradient for a Rod

The deformation gradient in this case is simply

$$\mathbf{F}(\xi) = 1 + \frac{\partial \mathbf{u}}{\partial \xi} \left(\frac{\partial \mathbf{x}_0}{\partial \xi} \right)^{-1} = 1 + \sum_{i=1}^2 N_{i,\xi} u_i \left(\sum_{i=1}^2 N_{i,\xi} x_{0i} \right)^{-1} = 1 + \frac{u_2 - u_1}{x_{02} - x_{01}} = \frac{x_2 - x_1}{x_{02} - x_{01}} \quad (3.2)$$

which is uniform over the length of a chord, i.e., it is independent of ξ .

3.2. 2D Triangles

Triangular elements are needed in a support capacity in order to construct our alevolar model; specifically, the four surfaces of a tetrahedron are triangles. What is required of them is a capability to compute the traction acting across such a surface through integration. This requires knowledge of their shape functions and quadrature rules, the latter of which is discussed in §5.

The shape functions for a triangle expressed in terms of its natural co-ordinates (ξ, η) , where $0 \leq \xi \leq 1$ and $0 \leq \eta \leq \xi$, are given by

$$N_1 = 1 - \xi - \eta \quad N_2 = \xi \quad N_3 = \eta \quad (3.3a)$$

with gradients of

$$N_{1,\xi} = -1 \quad N_{2,\xi} = 1 \quad N_{3,\xi} = 0 \quad (3.3b)$$

$$N_{2,\eta} = -1 \quad N_{2,\eta} = 0 \quad N_{3,\eta} = 1 \quad (3.3c)$$

so that the area of a triangle in its natural co-ordinates is $1/2$.

No further kinematics are required from triangular elements in our analysis.

3.3. 2D Irregular Pentagons

The kinematics of an irregular pentagon, on the other hand, are not trivial. Shape functions are required from which deformation gradients can then be constructed. Once a deformation gradient is in hand, the state of stretch occurring within a pentagon can finally be derived. Several possible decompositions of the deformation gradient are possible, i.e., stretch is not unique in 2D (nor in 3D). Here we employ the Laplace stretch [42].

3.3.1. Wachspress' Shape Functions for Interpolating an Irregular Pentagon

In 1975, Wachspress [43, 44] derived a set of shape functions N_i that are capable of interpolating convex polyhedra. His shape functions take on the form of rational polynomials, viz., $N_i = A_i/B$ where A_i and B are polynomials. In contrast, classic isoparametric elements are constructed from polynomial shape functions [45]. For the Wachspress shape functions of a pentagon, the A_i are cubic polynomials, while B is a quadratic polynomial.

Let us consider a convex pentagonal domain Ω defined over \mathbb{R}^2 whose vertices have global co-ordinates of

$$(x_1, y_1), (x_2, y_2), (x_3, y_3), (x_4, y_4), (x_5, y_5)$$

when evaluated in the pentagonal co-ordinate system $(\vec{\mathbf{e}}_1, \vec{\mathbf{e}}_2)$ of Fig. 2.5, with $\vec{\mathbf{e}}_3$ being an outward normal to the pentagon. Associated with this set of global co-ordinates is a set of local or natural co-ordinates

$$(\xi_1, \eta_1), (\xi_2, \eta_2), (\xi_3, \eta_3), (\xi_4, \eta_4), (\xi_5, \eta_5)$$

that describe a mapping or interpolation of

$$\begin{aligned} x(\xi, \eta) &= \sum_{i=1}^5 N_i(\xi, \eta) x_i \\ y(\xi, \eta) &= \sum_{i=1}^5 N_i(\xi, \eta) y_i \end{aligned} \quad \text{or} \quad \mathbf{x}(\boldsymbol{\xi}) = \sum_{i=1}^5 N_i(\boldsymbol{\xi}) \mathbf{x}_i \quad (3.4)$$

which relate natural co-ordinates $\boldsymbol{\xi} \equiv (\xi, \eta)$ to global co-ordinates $\mathbf{x} \equiv (x, y)$, where $\mathbf{x}_i \equiv (x_i, y_i)$ are nodal co-ordinates at the i^{th} vertex, with i indexing counterclockwise around a pentagon according to Fig. 2.2. Displacement $\mathbf{u}(\mathbf{x}) := \mathbf{x} - \mathbf{x}_0$, with reference co-ordinates $\mathbf{x}_0 \equiv (x_0, y_0)$, also obeys this mapping

$$\begin{aligned} u(\xi, \eta) &= \sum_{i=1}^5 N_i(\xi, \eta) u_i \\ v(\xi, \eta) &= \sum_{i=1}^5 N_i(\xi, \eta) v_i \end{aligned} \quad \text{or} \quad \mathbf{u}(\boldsymbol{\xi}) = \sum_{i=1}^5 N_i(\boldsymbol{\xi}) \mathbf{u}_i \quad (3.5)$$

whose co-ordinates $\mathbf{u}_i \equiv (u_i, v_i)$ designate the nodal displacements.

Shape functions $N_i(\boldsymbol{\xi}) \equiv N_i(\xi, \eta)$ are interpolation functions that place any position P with local co-ordinates $\boldsymbol{\xi} \equiv (\xi, \eta) \in \bar{\Omega}$, where $\bar{\Omega} := \Omega \cup \partial\Omega$, into their global co-ordinates $\mathbf{x} \equiv (x, y)$. The shape functions of Wachspress [43, 44] possess the following properties [46]:

1. Partition of unity: $\sum_{i=1}^5 N_i(\boldsymbol{\xi}) = 1$, $0 \leq N_i(\boldsymbol{\xi}) \leq 1$.
2. Interpolate nodal data: $N_i(\boldsymbol{\xi}_j) = \Xi_{ij}$.
3. Linear completeness: $\sum_{i=1}^5 N_i(\boldsymbol{\xi}) \mathbf{x}_i = \mathbf{x}$.
4. For $\boldsymbol{\xi} \in \Omega$, $N_i(\boldsymbol{\xi})$ is C^∞ , but for $\boldsymbol{\xi} \in \partial\Omega$, $N_i(\boldsymbol{\xi})$ is C^0 , i.e., interpolation is linear along an edge (or chord) connecting two neighboring vertices.

For interpolating a convex, planar, pentagonal shape, the shape functions of Wachspress have polynomials of order three in their numerators, and another polynomial of order two in their denominators; specifically, we write them here as

$$N_{i+1}(\xi, \eta) = \kappa_i A_i(\xi, \eta)/B(\xi, \eta), \quad i = 1, 2, \dots, 5 \quad (3.6a)$$

with scaling factors κ_i , where $N_1 \leftarrow N_6$, whose numerators and denominator for interpolating a pentagon are evaluated via

$$A_i(\xi, \eta) = \alpha_{0i} + \alpha_{1i}\xi + \alpha_{2i}\eta + \alpha_{3i}\xi^2 + \alpha_{4i}\xi\eta + \alpha_{5i}\eta^2 + \alpha_{6i}\xi^3 + \alpha_{7i}\xi^2\eta + \alpha_{8i}\xi\eta^2 + \alpha_{9i}\eta^3 \quad (3.6b)$$

$$B(\xi, \eta) = \beta_0 + \beta_1\xi + \beta_2\eta + \beta_3\xi^2 + \beta_4\xi\eta + \beta_5\eta^2 \quad (3.6c)$$

where coefficients in the numerator, i.e., A_i , differ with index i , while those in the denominator, viz., $B := \sum_{i=1}^5 A_i$, are the same for all five shape functions.

We apply the construction technique of Dasgupta [47] to compute the shape functions of Wachspress for an irregular convex pentagon. Consider a chord c_i that connects vertex

$\xi_{i-1} = (\xi_{i-1}, \eta_{i-1})$ with vertex $\xi_i = (\xi_i, \eta_i)$ via a straight line segment such that $\ell_i = 0$ with $\ell_i := 1 - a_i \xi - b_i \eta$ wherein

$$a_i = \frac{\eta_i - \eta_{i-1}}{\xi_{i-1}\eta_i - \xi_i\eta_{i-1}} \quad (3.7a)$$

$$b_i = \frac{\xi_{i-1} - \xi_i}{\xi_{i-1}\eta_i - \xi_i\eta_{i-1}} \quad (3.7b)$$

for which Dasgupta derived the following set of constraints

$$\kappa_i = \kappa_{i-1} \left(\frac{a_{i+1}(\xi_{i-1} - \xi_i) + b_{i+1}(\eta_{i-1} - \eta_i)}{a_{i-1}(\xi_i - \xi_{i-1}) + b_{i-1}(\eta_i - \eta_{i-1})} \right) \quad (3.7c)$$

with recursion starting at $\kappa_1 := 1$. Coefficients κ_i enforce property 4 listed above.

With this information in hand, we derived the rational polynomials describing Wachspress' shape functions for a pentagon specified in Eq. (3.6) in terms of parameters a_i , b_i and κ_i . The polynomial coefficients for the A_i in Eq. (3.6b) have values of

$$\alpha_{0i} = 1 \quad (3.8a)$$

$$\alpha_{1i} = -(a_{i+1} + a_{i+2} + a_{i+3}) \quad (3.8b)$$

$$\alpha_{2i} = -(b_{i+1} + b_{i+2} + b_{i+3}) \quad (3.8c)$$

$$\alpha_{3i} = a_{i+1}a_{i+2} + a_{i+2}a_{i+3} + a_{i+3}a_{i+1} \quad (3.8d)$$

$$\alpha_{4i} = a_{i+1}(b_{i+2} + b_{i+3}) + a_{i+2}(b_{i+1} + b_{i+3}) + a_{i+3}(b_{i+1} + b_{i+2}) \quad (3.8e)$$

$$\alpha_{5i} = b_{i+1}b_{i+2} + b_{i+2}b_{i+3} + b_{i+3}b_{i+1} \quad (3.8f)$$

$$\alpha_{6i} = -a_{i+1}a_{i+2}a_{i+3} \quad (3.8g)$$

$$\alpha_{7i} = -(a_{i+1}a_{i+2}b_{i+3} + a_{i+1}b_{i+2}a_{i+3} + b_{i+1}a_{i+2}a_{i+3}) \quad (3.8h)$$

$$\alpha_{8i} = -(a_{i+1}b_{i+2}b_{i+3} + b_{i+1}a_{i+2}b_{i+3} + b_{i+1}b_{i+2}a_{i+3}) \quad (3.8i)$$

$$\alpha_{9i} = -b_{i+1}b_{i+2}b_{i+3} \quad (3.8j)$$

which differ for each shape function via index $i = 1, 2, \dots, 5$, while the polynomial coefficients for B in Eq. (3.6c) have values of

$$\beta_i = \sum_{j=1}^5 \alpha_{ij} \kappa_j, \quad i = 0, 1, \dots, 5 \quad (3.9)$$

which are the same for all five shape functions. Sums over the four cubic terms in Eq. (3.8) all vanish—a byproduct of Wachspress' formulation. In the above formulæ, an index count of $i \equiv 0 \implies i = 5$, while index counts of $i \equiv 6 \implies i = 1$, $i \equiv 7 \implies i = 2$ and $i \equiv 8 \implies i = 3$. Shape function N_1 is illustrated in Fig. 3.1, with like images applying for the other four shape functions.

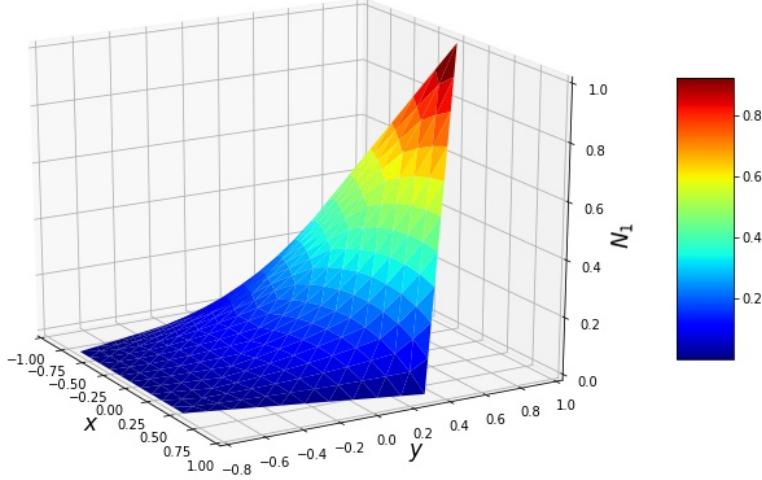


Figure 3.1: Wachspress shape functions for a pentagon, in this case, shape function N_1 .

3.3.2. Spatial Derivatives of Shape Functions

The first derivatives of Wachspress' shape functions for a pentagon are

$$N_{i+1,\xi}(\xi, \eta) = \kappa_i \mathcal{N}_{i,\xi}(\xi, \eta) / B^2(\xi, \eta) \quad (3.10a)$$

$$N_{i+1,\eta}(\xi, \eta) = \kappa_i \mathcal{N}_{i,\eta}(\xi, \eta) / B^2(\xi, \eta) \quad (3.10b)$$

where $N_{i+1,\xi}(\xi, \eta) = \partial N_{i+1}(\xi, \eta) / \partial \xi$ and $N_{i+1,\eta}(\xi, \eta) = \partial N_{i+1}(\xi, \eta) / \partial \eta$ with

$$\mathcal{N}_{i,\xi}(\xi, \eta) = B(\xi, \eta) A_{i,\xi}(\xi, \eta) - B_{,\xi}(\xi, \eta) A_i(\xi, \eta) \quad (3.10c)$$

$$\mathcal{N}_{i,\eta}(\xi, \eta) = B(\xi, \eta) A_{i,\eta}(\xi, \eta) - B_{,\eta}(\xi, \eta) A_i(\xi, \eta) \quad (3.10d)$$

which contain the polynomials

$$A_{i,\xi}(\xi, \eta) = \alpha_{1i} + 2\alpha_{3i}\xi + \alpha_{4i}\eta + 3\alpha_{6i}\xi^2 + 2\alpha_{7i}\xi\eta + \alpha_{8i}\eta^2 \quad (3.10e)$$

$$A_{i,\eta}(\xi, \eta) = \alpha_{2i} + \alpha_{4i}\xi + 2\alpha_{5i}\eta + \alpha_{7i}\xi^2 + 2\alpha_{8i}\xi\eta + 3\alpha_{9i}\eta^2 \quad (3.10f)$$

$$B_{,\xi}(\xi, \eta) = \beta_1 + 2\beta_3\xi + \beta_4\eta \quad (3.10g)$$

$$B_{,\eta}(\xi, \eta) = \beta_2 + \beta_4\xi + 2\beta_5\eta \quad (3.10h)$$

from which the deformation and displacement gradients are constructed.

The second derivatives of these shape functions, which we used to test the compatibility conditions of this element, are described by

$$N_{i+1,\xi\xi} = \kappa_i \mathfrak{N}_{i,\xi\xi}(\xi, \eta) / B^3(\xi, \eta) \quad (3.11a)$$

$$N_{i+1,\xi\eta} = \kappa_i \mathfrak{N}_{i,\xi\eta}(\xi, \eta) / B^3(\xi, \eta) \quad (3.11b)$$

$$N_{i+1,\eta\xi} = \kappa_i \mathfrak{N}_{i,\eta\xi}(\xi, \eta) / B^3(\xi, \eta) \quad (3.11c)$$

$$N_{i+1,\eta\eta} = \kappa_i \mathfrak{N}_{i,\eta\eta}(\xi, \eta) / B^3(\xi, \eta) \quad (3.11d)$$

where $N_{i+1,\xi\eta}(\xi, \eta) = \partial^2 N_{i+1}(\xi, \eta) / \partial \xi \partial \eta$, etc., and where

$$\mathfrak{N}_{i,\xi\xi}(\xi, \eta) = B(\xi, \eta) \mathcal{N}_{i,\xi\xi}(\xi, \eta) - 2B_{,\xi}(\xi, \eta) \mathcal{N}_{i,\xi}(\xi, \eta) \quad (3.11e)$$

$$\mathfrak{N}_{i,\xi\eta}(\xi, \eta) = B(\xi, \eta) \mathcal{N}_{i,\xi\eta}(\xi, \eta) - 2B_{,\xi}(\xi, \eta) \mathcal{N}_{i,\eta}(\xi, \eta) \quad (3.11f)$$

$$\mathfrak{N}_{i,\eta\xi}(\xi, \eta) = B(\xi, \eta) \mathcal{N}_{i,\eta\xi}(\xi, \eta) - 2B_{,\eta}(\xi, \eta) \mathcal{N}_{i,\xi}(\xi, \eta) \quad (3.11g)$$

$$\mathfrak{N}_{i,\eta\eta}(\xi, \eta) = B(\xi, \eta) \mathcal{N}_{i,\eta\eta}(\xi, \eta) - 2B_{,\eta}(\xi, \eta) \mathcal{N}_{i,\eta}(\xi, \eta) \quad (3.11h)$$

wherein

$$\mathcal{N}_{i,\xi\xi}(\xi, \eta) = B(\xi, \eta) A_{i,\xi\xi}(\xi, \eta) - B_{,\xi\xi}(\xi, \eta) A_i(\xi, \eta) \quad (3.11i)$$

$$\begin{aligned} \mathcal{N}_{i,\xi\eta}(\xi, \eta) &= B(\xi, \eta) A_{i,\xi\eta}(\xi, \eta) + B_{,\xi}(\xi, \eta) A_{i,\eta}(\xi, \eta) \\ &\quad - B_{,\eta}(\xi, \eta) A_{i,\xi}(\xi, \eta) - B_{,\xi\eta}(\xi, \eta) A_i(\xi, \eta) \end{aligned} \quad (3.11j)$$

$$\begin{aligned} \mathcal{N}_{i,\eta\xi}(\xi, \eta) &= B(\xi, \eta) A_{i,\eta\xi}(\xi, \eta) + B_{,\eta}(\xi, \eta) A_{i,\xi}(\xi, \eta) \\ &\quad - B_{,\xi}(\xi, \eta) A_{i,\eta}(\xi, \eta) - B_{,\eta\xi}(\xi, \eta) A_i(\xi, \eta) \end{aligned} \quad (3.11k)$$

$$\mathcal{N}_{i,\eta\eta}(\xi, \eta) = B(\xi, \eta) A_{i,\eta\eta}(\xi, \eta) - B_{,\eta\eta}(\xi, \eta) A_i(\xi, \eta) \quad (3.11l)$$

which contain polynomials

$$A_{i,\xi\xi}(\xi, \eta) = 2\alpha_{3i} + 6\alpha_{6i}\xi + 2\alpha_{7i}\eta \quad (3.11m)$$

$$A_{i,\xi\eta}(\xi, \eta) = \alpha_{4i} + 2\alpha_{7i}\xi + 2\alpha_{8i}\eta \quad (3.11n)$$

$$A_{i,\eta\eta}(\xi, \eta) = 2\alpha_{5i} + 2\alpha_{8i}\xi + 6\alpha_{9i}\eta \quad (3.11o)$$

$$B_{,\xi\xi}(\xi, \eta) = 2\beta_3 \quad (3.11p)$$

$$B_{,\xi\eta}(\xi, \eta) = \beta_4 \quad (3.11q)$$

$$B_{,\eta\eta}(\xi, \eta) = 2\beta_5 \quad (3.11r)$$

with $A_{i,\xi\eta}(\xi, \eta) = A_{i,\eta\xi}(\xi, \eta)$ and $B_{,\xi\eta}(\xi, \eta) = B_{,\eta\xi}(\xi, \eta)$.

3.3.3. Deformation Gradient for an Irregular Pentagon

Derivatives of displacement (u, v) taken with respect to the local co-ordinates (ξ, η) used to describe the shape functions $N_i(\xi, \eta)$ of a pentagon result in a local displacement gradient with components

$$\begin{bmatrix} \partial u / \partial \xi & \partial u / \partial \eta \\ \partial v / \partial \xi & \partial v / \partial \eta \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^5 N_{i,\xi}(\xi, \eta) u_i & \sum_{i=1}^5 N_{i,\eta}(\xi, \eta) u_i \\ \sum_{i=1}^5 N_{i,\xi}(\xi, \eta) v_i & \sum_{i=1}^5 N_{i,\eta}(\xi, \eta) v_i \end{bmatrix} \quad (3.12a)$$

where $u := x - x_0$ and $v := y - y_0$. Gradients of the global co-ordinates (x_0, y_0) evaluated in a reference state taken with respect to local co-ordinates (ξ, η) are described by the matrix equation

$$\begin{bmatrix} \partial x_0 / \partial \xi & \partial x_0 / \partial \eta \\ \partial y_0 / \partial \xi & \partial y_0 / \partial \eta \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^5 N_{i,\xi}(\xi, \eta) x_{0i} & \sum_{i=1}^5 N_{i,\eta}(\xi, \eta) x_{0i} \\ \sum_{i=1}^5 N_{i,\xi}(\xi, \eta) y_{0i} & \sum_{i=1}^5 N_{i,\eta}(\xi, \eta) y_{0i} \end{bmatrix} \quad (3.12b)$$

wherein (x_{0i}, y_{0i}) are the reference global co-ordinates at the i^{th} vertex, while gradients of the global co-ordinates (x, y) evaluated in the current state taken with respect to local co-ordinates (ξ, η) are described by the matrix equation

$$\mathbf{J} := \begin{bmatrix} \partial x / \partial \xi & \partial x / \partial \eta \\ \partial y / \partial \xi & \partial y / \partial \eta \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^5 N_{i,\xi}(\xi, \eta) x_i & \sum_{i=1}^5 N_{i,\eta}(\xi, \eta) x_i \\ \sum_{i=1}^5 N_{i,\xi}(\xi, \eta) y_i & \sum_{i=1}^5 N_{i,\eta}(\xi, \eta) y_i \end{bmatrix} \quad (3.12c)$$

wherein (x_i, y_i) are the current global co-ordinates at the i^{th} vertex, with \mathbf{J} being the Jacobian matrix.

From the above matrices, one can construct the deformation gradient $\mathbf{F} = \partial \mathbf{x} / \partial \mathbf{x}_0 = \mathbf{I} + \partial \mathbf{u} / \partial \mathbf{x}_0$ for an irregular pentagon via

$$\mathbf{F}(\xi, \eta) = \begin{bmatrix} F_{11}(\xi, \eta) & F_{12}(\xi, \eta) \\ F_{21}(\xi, \eta) & F_{22}(\xi, \eta) \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} \partial u / \partial \xi & \partial u / \partial \eta \\ \partial v / \partial \xi & \partial v / \partial \eta \end{bmatrix} \begin{bmatrix} \partial x_0 / \partial \xi & \partial x_0 / \partial \eta \\ \partial y_0 / \partial \xi & \partial y_0 / \partial \eta \end{bmatrix}^{-1} \quad (3.13a)$$

whose inverse is

$$\mathbf{F}^{-1}(\xi, \eta) = \frac{1}{F_{11}(\xi, \eta)F_{22}(\xi, \eta) - F_{21}(\xi, \eta)F_{12}(\xi, \eta)} \begin{bmatrix} F_{22}(\xi, \eta) & -F_{12}(\xi, \eta) \\ -F_{21}(\xi, \eta) & F_{11}(\xi, \eta) \end{bmatrix} \quad (3.13b)$$

while its associated displacement gradient $\mathbf{G} = \partial \mathbf{u} / \partial \mathbf{x}$ follows from

$$\mathbf{G}(\xi, \eta) = \begin{bmatrix} G_{11}(\xi, \eta) & G_{12}(\xi, \eta) \\ G_{21}(\xi, \eta) & G_{22}(\xi, \eta) \end{bmatrix} = \begin{bmatrix} \partial u / \partial \xi & \partial u / \partial \eta \\ \partial v / \partial \xi & \partial v / \partial \eta \end{bmatrix} \begin{bmatrix} \partial x / \partial \xi & \partial x / \partial \eta \\ \partial y / \partial \xi & \partial y / \partial \eta \end{bmatrix}^{-1} \quad (3.14)$$

which is not invertible, in general. All are evaluated in the 12 plane belonging to a co-ordinate system $(\vec{\mathbf{e}}_1, \vec{\mathbf{e}}_2, \vec{\mathbf{e}}_3)$ that orients this pentagon, with $\vec{\mathbf{e}}_3$ being normal to its surface, as illustrated in Fig. 2.5. The deformation and displacement gradients are two, fundamental, kinematic fields commonly used in the construction of constitutive equations. They are exported as methods from module `shapeFunctions` described in Appendix F.1 along with the velocity gradient $\mathbf{L}(\xi, \eta) = \dot{\mathbf{F}}(\xi, \eta) \mathbf{F}^{-1}(\xi, \eta)$.

3.3.4. Compatibility Conditions

To ensure that a deformation is compatible, and therefore integrable, it follows that the curl of its deformation gradient must be zero [48]. This condition is trivially satisfied for the shape functions that we use for 1D chords, 2D triangles, and 3D tetrahedra. However,

for the Wachspress shape function used to interpolate pentagons, this needs to be verified. Vanishing of the curl of \mathbf{F} results in two constraint equations for the planar case, they being

$$F_{11,2} = F_{12,1} \quad \text{and} \quad F_{22,1} = F_{21,2} \quad (3.15)$$

whose spatial derivatives associate with the $(\vec{\mathbf{e}}_1, \vec{\mathbf{e}}_2)$ co-ordinate frame.

From Eqn. (3.13), it follows that the spatial derivatives of the deformation gradient are

$$\begin{aligned} \mathbf{F}_{,1}(\xi, \eta) &= \frac{\partial}{\partial x_0} \begin{bmatrix} F_{11}(\xi, \eta) & F_{12}(\xi, \eta) \\ F_{21}(\xi, \eta) & F_{22}(\xi, \eta) \end{bmatrix} \\ &= \frac{\partial \xi}{\partial x_0} \left(\frac{\partial}{\partial \xi} \begin{bmatrix} \partial u / \partial \xi & \partial u / \partial \eta \\ \partial v / \partial \xi & \partial v / \partial \eta \end{bmatrix} \right) \begin{bmatrix} \partial x_0 / \partial \xi & \partial x_0 / \partial \eta \\ \partial y_0 / \partial \xi & \partial y_0 / \partial \eta \end{bmatrix}^{-1} - \begin{bmatrix} \partial u / \partial \xi & \partial u / \partial \eta \\ \partial v / \partial \xi & \partial v / \partial \eta \end{bmatrix} \\ &\quad \times \begin{bmatrix} \partial x_0 / \partial \xi & \partial x_0 / \partial \eta \\ \partial y_0 / \partial \xi & \partial y_0 / \partial \eta \end{bmatrix}^{-1} \frac{\partial}{\partial \xi} \left(\begin{bmatrix} \partial x_0 / \partial \xi & \partial x_0 / \partial \eta \\ \partial y_0 / \partial \xi & \partial y_0 / \partial \eta \end{bmatrix} \right) \begin{bmatrix} \partial x_0 / \partial \xi & \partial x_0 / \partial \eta \\ \partial y_0 / \partial \xi & \partial y_0 / \partial \eta \end{bmatrix}^{-1} \end{aligned} \quad (3.16a)$$

and

$$\begin{aligned} \mathbf{F}_{,2}(\xi, \eta) &= \frac{\partial}{\partial y_0} \begin{bmatrix} F_{11}(\xi, \eta) & F_{12}(\xi, \eta) \\ F_{21}(\xi, \eta) & F_{22}(\xi, \eta) \end{bmatrix} \\ &= \frac{\partial \eta}{\partial y_0} \left(\frac{\partial}{\partial \eta} \begin{bmatrix} \partial u / \partial \xi & \partial u / \partial \eta \\ \partial v / \partial \xi & \partial v / \partial \eta \end{bmatrix} \right) \begin{bmatrix} \partial x_0 / \partial \xi & \partial x_0 / \partial \eta \\ \partial y_0 / \partial \xi & \partial y_0 / \partial \eta \end{bmatrix}^{-1} - \begin{bmatrix} \partial u / \partial \xi & \partial u / \partial \eta \\ \partial v / \partial \xi & \partial v / \partial \eta \end{bmatrix} \\ &\quad \times \begin{bmatrix} \partial x_0 / \partial \xi & \partial x_0 / \partial \eta \\ \partial y_0 / \partial \xi & \partial y_0 / \partial \eta \end{bmatrix}^{-1} \frac{\partial}{\partial \eta} \left(\begin{bmatrix} \partial x_0 / \partial \xi & \partial x_0 / \partial \eta \\ \partial y_0 / \partial \xi & \partial y_0 / \partial \eta \end{bmatrix} \right) \begin{bmatrix} \partial x_0 / \partial \xi & \partial x_0 / \partial \eta \\ \partial y_0 / \partial \xi & \partial y_0 / \partial \eta \end{bmatrix}^{-1} \end{aligned} \quad (3.16b)$$

wherein

$$\frac{\partial}{\partial \xi} \begin{bmatrix} \partial u / \partial \xi & \partial u / \partial \eta \\ \partial v / \partial \xi & \partial v / \partial \eta \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^5 N_{i,\xi\xi}(\xi, \eta) u_i & \sum_{i=1}^5 N_{i,\xi\eta}(\xi, \eta) u_i \\ \sum_{i=1}^5 N_{i,\xi\xi}(\xi, \eta) v_i & \sum_{i=1}^5 N_{i,\xi\eta}(\xi, \eta) v_i \end{bmatrix} \quad (3.17a)$$

$$\frac{\partial}{\partial \eta} \begin{bmatrix} \partial u / \partial \xi & \partial u / \partial \eta \\ \partial v / \partial \xi & \partial v / \partial \eta \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^5 N_{i,\eta\xi}(\xi, \eta) u_i & \sum_{i=1}^5 N_{i,\eta\eta}(\xi, \eta) u_i \\ \sum_{i=1}^5 N_{i,\eta\xi}(\xi, \eta) v_i & \sum_{i=1}^5 N_{i,\eta\eta}(\xi, \eta) v_i \end{bmatrix} \quad (3.17b)$$

and

$$\frac{\partial}{\partial \xi} \begin{bmatrix} \partial x_0 / \partial \xi & \partial x_0 / \partial \eta \\ \partial y_0 / \partial \xi & \partial y_0 / \partial \eta \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^5 N_{i,\xi\xi}(\xi, \eta) x_{0i} & \sum_{i=1}^5 N_{i,\xi\eta}(\xi, \eta) x_{0i} \\ \sum_{i=1}^5 N_{i,\xi\xi}(\xi, \eta) y_{0i} & \sum_{i=1}^5 N_{i,\xi\eta}(\xi, \eta) y_{0i} \end{bmatrix} \quad (3.17c)$$

$$\frac{\partial}{\partial \eta} \begin{bmatrix} \partial x_0 / \partial \xi & \partial x_0 / \partial \eta \\ \partial y_0 / \partial \xi & \partial y_0 / \partial \eta \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^5 N_{i,\eta\xi}(\xi, \eta) x_{0i} & \sum_{i=1}^5 N_{i,\eta\eta}(\xi, \eta) x_{0i} \\ \sum_{i=1}^5 N_{i,\eta\xi}(\xi, \eta) y_{0i} & \sum_{i=1}^5 N_{i,\eta\eta}(\xi, \eta) y_{0i} \end{bmatrix} \quad (3.17d)$$

with $\partial \xi / \partial x_0$ and $\partial \eta / \partial y_0$ effectively being scaling factors that we take to be described as a ratio of septal chord lengths; specifically, let

$$\frac{\partial \xi}{\partial x_0} \approx \frac{\partial \eta}{\partial y_0} \approx \frac{L(\xi, \eta)}{L_0(x, y)} = \frac{\cos(\omega)}{\sqrt{A_0/5 \tan(\omega)}} \quad (3.18)$$

where $L(\xi, \eta)$ is the septal length of a pentagonal edge in its natural configuration, as drawn in Fig. 2.2, while $L_0(x, y)$ is the actual, alveolar, septal length with $A_0(x, y)$ being the area of an alveolar septum in its reference state. This formula follows from Eqns. (2.5 & 2.6).

We study compatibility only for the purpose of assessing applicability in our choice of selecting Wachspress shape functions. Otherwise, it is not required from our modeling of an alveolus via a dodecahedron.

3.3.5. Gram-Schmidt Decomposition of the Deformation Gradient

To describe the kinematics of a planar membrane, an upper-triangular Gram-Schmidt decomposition of the deformation gradient \mathbf{F} is used in lieu of the symmetric polar decomposition that is commonly adopted [42, 49–52]. McLellan [38, 53] was the first to propose a triangular decomposition of \mathbf{F} , to prove its uniqueness and existence, and to establish many of its physical properties. This idea has been rediscovered several times since then, e.g., [49, 54, 55]. A thorough history of the **QR** (Gram-Schmidt) decomposition has been written by Leon, Björck and Gander [56], with a brief history regarding its application to kinematics being given in Ref. [42].

A Gram-Schmidt factorization of the deformation gradient \mathbf{F} is written here as $\mathbf{F} = \mathcal{R}\mathcal{U}$, where the rotation \mathcal{R} is orthogonal, and where the Laplace stretch \mathcal{U} is upper-triangular [42].⁴ This triangular measure of stretch possesses an inherent property in two space: the direction aligned with the rotated 1-axis, denoted as $\vec{\mathbf{g}}_1$, remains invariant under transformation \mathcal{U} [38], i.e., it is a material vector in a neighborhood surrounding that particle whereat \mathbf{F} is evaluated [39]. This property has some interesting ramifications addressed in §3.3.5.2.

3.3.5.1. **QR** Factorization of \mathbf{F}

The 2×2 deformation gradient associated with a planar membrane has a Gram-Schmidt decomposition expressed in terms of four physical attributes. Three of these attributes describe deformation. They are defined as [51]

$$a = \sqrt{F_{11}^2 + F_{21}^2}, \quad b = \frac{F_{11}F_{22} - F_{12}F_{21}}{\sqrt{F_{11}^2 + F_{21}^2}}, \quad g = \frac{F_{11}F_{12} + F_{22}F_{21}}{F_{11}^2 + F_{21}^2} \quad (3.19)$$

thereby populating Laplace stretch \mathcal{U} and its inverse \mathcal{U}^{-1} with components

$$\mathcal{U} = \begin{bmatrix} a & ag \\ 0 & b \end{bmatrix} \quad \text{and} \quad \mathcal{U}^{-1} = \begin{bmatrix} 1/a & -g/b \\ 0 & 1/b \end{bmatrix} \quad (3.20)$$

where a and b are the principal elongations (ratios of current lengths to reference lengths) and g is the extent of in-plane shear, as measured in a co-ordinate frame $(\vec{\mathbf{g}}_1, \vec{\mathbf{g}}_2)$ illustrated in Fig. 3.2. It is worth pointing out that the components of Laplace stretch, viz., \mathcal{U}_{ij} , are evaluated in the reference co-ordinate system $(\vec{\mathbf{e}}_1, \vec{\mathbf{e}}_2)$ of the pentagon, as $\mathbf{F} = F_{ij} \vec{\mathbf{e}}_i \otimes \vec{\mathbf{e}}_j$, but their physical interpretations arise in co-ordinate system $(\vec{\mathbf{g}}_1, \vec{\mathbf{g}}_2)$.

⁴The **QR** rotation \mathcal{R} and stretch \mathcal{U} tensors are distinct from those that arise from a polar decomposition of a deformation gradient, typically denoted as \mathbf{R} and \mathbf{U} , as found in any, modern, continuum mechanics text. McLellan [38, 53] introduced the Laplace stretch in 1976, which he denoted as \mathbf{H} , while Srinivasa [49] denoted it as $\tilde{\mathbf{F}}$ in his 2012 paper.

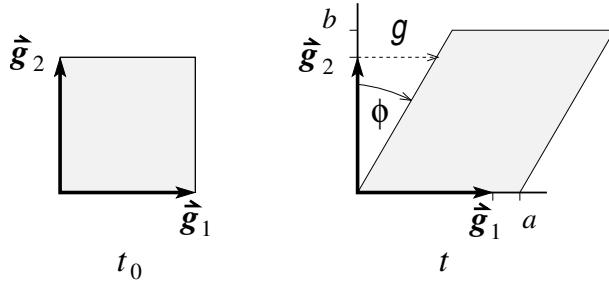


Figure 3.2: Physical attributes of a planar deformation: a and b represent elongations, while $g = \tan \phi$ denotes the extent of shear. They are measured in a physical frame of reference with unit base vectors (\vec{g}_1, \vec{g}_2) where \vec{g}_1 embeds in the material.

An orthogonal tensor $\mathcal{R} = [\vec{g}_1 \mid \vec{g}_2] = \delta_{ij} \vec{g}_i \otimes \vec{e}_j = \mathcal{R}_{ij} \vec{e}_i \otimes \vec{e}_j$ rotates the reference coordinate axes (\vec{e}_1, \vec{e}_2) into a physical coordinate system (\vec{g}_1, \vec{g}_2) through an angle θ , which is the fourth physical attribute arising from a **QR** factorization of \mathbf{F} . This angle of rotation describes an orthogonal matrix whereby

$$\mathcal{R} = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix} \quad (3.21)$$

with

$$\sin \theta = \frac{F_{21}}{\sqrt{F_{11}^2 + F_{21}^2}}, \quad \cos \theta = \frac{F_{11}}{\sqrt{F_{11}^2 + F_{21}^2}} \quad \therefore \quad \theta = \tan^{-1} \left(\frac{F_{21}}{F_{11}} \right) \quad (3.22)$$

where a positive angle θ corresponds with a counterclockwise rotation of physical axes (\vec{g}_1, \vec{g}_2) about reference axes (\vec{e}_1, \vec{e}_2) .

3.3.5.2. Dilemma

Until recently, there has been a tacit assumption in prior applications of Gram-Schmidt factorizations of \mathbf{F} that the physical base vectors (\vec{g}_1, \vec{g}_2) always satisfy a geometric condition whereby the physical 1-direction \vec{g}_1 rotates out of the reference 1-direction \vec{e}_1 , but this need not always be the case. Physical vector \vec{g}_1 could equally likely rotate out of the 2-direction \vec{e}_2 of the reference frame. At issue is not: How the physical base vectors orient in space? That is managed by Gram's procedure. Rather, at issue is: How do the physical base vectors index with respect to the reference base vectors?

To illustrate this concern, consider two deformation histories, as drawn in Fig. 3.3, each of which describe a simple shear taking place in the plane of a membrane. In one case shear occurs in the 1-direction, while in the other case shear occurs in the 2-direction. There are no elongations in this deformation. These motions lead to Gram-Schmidt factorizations of the deformation gradient, when following the protocol of Eqns. (3.19–3.22), that are described by

$$\mathbf{F} = \begin{bmatrix} 1 & \gamma \\ 0 & 1 \end{bmatrix} \implies \mathcal{R} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathcal{U} = \begin{bmatrix} 1 & \gamma \\ 0 & 1 \end{bmatrix} \quad (3.23a)$$

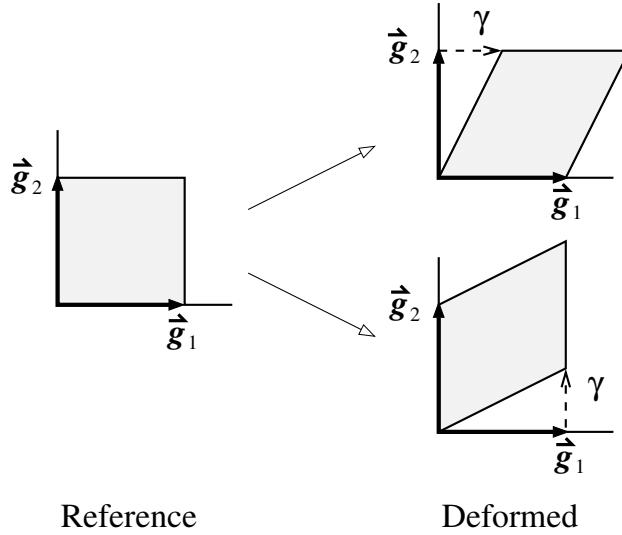


Figure 3.3: The left graphic designates a reference configuration while the right two graphics designate deformed configurations, both in basis (\vec{g}_1, \vec{g}_2) . The top graphic associates with the motion of Eqn. (3.23a), while the bottom graphic associates with the motion of Eqn. (3.23b).

and

$$\mathbf{F} = \begin{bmatrix} 1 & 0 \\ \gamma & 1 \end{bmatrix} \implies \begin{cases} \mathcal{R} = \frac{1}{\sqrt{1+\gamma^2}} \begin{bmatrix} 1 & -\gamma \\ \gamma & 1 \end{bmatrix} \\ \mathcal{U} = \begin{bmatrix} \sqrt{1+\gamma^2} & \gamma \\ 0 & 1/\sqrt{1+\gamma^2} \end{bmatrix} \end{cases} \quad (3.23b)$$

where we see that shear \mathcal{U}_{12} has the same physical interpretation in both cases, viz., γ , but the elongations \mathcal{U}_{11} and \mathcal{U}_{22} do not, viz., $\mathcal{U}_{11} = 1$ and $\mathcal{U}_{22} = 1$ in Eq. (3.23a), whereas $\mathcal{U}_{11} = \sqrt{1+\gamma^2}$ and $\mathcal{U}_{22} = 1/\sqrt{1+\gamma^2}$ for the motion described in Eq. (3.23b). Consequently, two geometric interpretations are produced for just one physical mode of deformation. This cannot be!

The only difference between the motions that lead to the two deformation gradients presented in Eq. (3.23) is one's choice for labeling the co-ordinate directions. Matrix operations of row and column pivoting, taken from linear algebra, allow one to transform the lower-triangular form of Eq. (3.23b) into an upper-triangular form like Eq. (3.23a); hence, producing an unified physical interpretation for both shearing motions, and thereby providing a means for establishing a remedy to this dilemma.

3.3.5.3. Remedy

For 2D membranes, there are only two co-ordinate re-indexings that are possible (for 3D solids there are six, cf. §2.1). The default is no re-indexing at all, in which case

$$[\mathbf{P}] = [\mathbf{P}_0] := \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \implies \begin{bmatrix} \mathcal{F}_{11} & \mathcal{F}_{12} \\ \mathcal{F}_{21} & \mathcal{F}_{22} \end{bmatrix} := \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix} \quad (3.24a)$$

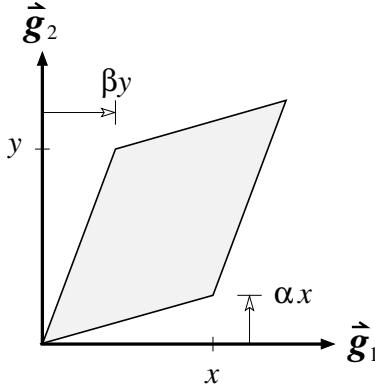


Figure 3.4: A general description for uniform planar deformation, where $x, y \in \mathbb{R}_+$ and $\alpha, \beta \in \mathbb{R}$. Shears α and β are drawn in their positive sense.

while in the second case there is a re-indexing specified by

$$[\mathbf{P}] = [\mathbf{P}_1] := \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \Rightarrow \quad \begin{bmatrix} \mathcal{F}_{11} & \mathcal{F}_{12} \\ \mathcal{F}_{21} & \mathcal{F}_{22} \end{bmatrix} := \begin{bmatrix} F_{22} & F_{21} \\ F_{12} & F_{11} \end{bmatrix} \quad (3.24b)$$

where components $\mathcal{F}_{ij} = P_{ki}F_{k\ell}P_{\ell j}$ are the components to be used in the Gram-Schmidt factorization presented in §3.3.5.1, and where $\mathbf{P} \in \{\mathbf{P}_0, \mathbf{P}_1\}$ is orthogonal, i.e., $\mathbf{P}\mathbf{P}^T = \mathbf{P}^T\mathbf{P} = \mathbf{I}$ with $\det \mathbf{P} = \pm 1$; specifically, $\det \mathbf{P}_0 = +1$ while $\det \mathbf{P}_1 = -1$.

The challenge in implementing such a strategy is to determine when to switch from \mathbf{P}_0 (case 1) to \mathbf{P}_1 (case 2), or back again, viz., from \mathbf{P}_1 to \mathbf{P}_0 . Continuity in the physical fields of deformation (a, b, g) must be satisfied in order for such a change in co-ordinate frame to be physically meaningful. To this end, it is useful to represent the components of a planar deformation gradient as

$$\begin{bmatrix} \mathcal{F}_{11} & \mathcal{F}_{12} \\ \mathcal{F}_{21} & \mathcal{F}_{22} \end{bmatrix} = \begin{cases} \text{case 1 : } & \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix} = \begin{bmatrix} x & \beta y \\ \alpha x & y \end{bmatrix} \\ \text{case 2 : } & \begin{bmatrix} F_{22} & F_{21} \\ F_{12} & F_{11} \end{bmatrix} = \begin{bmatrix} y & \alpha x \\ \beta y & x \end{bmatrix} \end{cases} \quad (3.25)$$

where $x = F_{11}$ and $y = F_{22}$ are elongations, while ratios $\alpha = F_{21}/F_{11}$ and $\beta = F_{12}/F_{22}$ are magnitudes of shear, as illustrated in Fig. 3.4.

The physical attributes for Laplace stretch, as they pertain to the two cases in Eqn. (3.24), written in terms of components F_{ij} from $\mathbf{F} = F_{ij} \vec{\mathbf{e}}_i \otimes \vec{\mathbf{e}}_j$ as defined in Eqn. (3.25), are respectively given by

$$\tilde{a} = x\sqrt{1 + \alpha^2} \quad \hat{a} = y\sqrt{1 + \beta^2} \quad (3.26a)$$

$$\tilde{b} = y(1 - \alpha\beta) / \sqrt{1 + \alpha^2} \quad \hat{b} = x(1 - \alpha\beta) / \sqrt{1 + \beta^2} \quad (3.26b)$$

$$\tilde{g} = y(\alpha + \beta) / x(1 + \alpha^2) \quad \hat{g} = x(\alpha + \beta) / y(1 + \beta^2) \quad (3.26c)$$

$$\tilde{\theta} = \tan^{-1}(-\alpha) \quad \hat{\theta} = \tan^{-1}(-\beta) \quad (3.26d)$$

where attributes in the left column apply to case 1 (i.e., Eqn. 3.24a) while those in the right column apply to case 2 (viz., Eqn. 3.24b). The actual set of physical attributes $\{a, b, g, \theta\}$ that are to be used when quantifying Laplace stretch and its inverse, according to Eqn. (4.38), are then selected via the strategy

$$\text{if } |\tilde{g}| \geq |\hat{g}| : \quad \{\tilde{a}, \tilde{b}, \tilde{g}, \tilde{\theta}\} \mapsto \{a, b, g, \theta\} \quad (3.27a)$$

$$\text{else } |\tilde{g}| \leq |\hat{g}| : \quad \{\hat{a}, \hat{b}, \hat{g}, \hat{\theta}\} \mapsto \{a, b, g, \theta\} \quad (3.27b)$$

where it is easily verified that $\tilde{a} = \hat{a}$ and $\tilde{b} = \hat{b}$ whenever $\tilde{g} = \hat{g}$; consequently, the physical attributes of deformation a, b, g remain continuous across a co-ordinate switch, however, the angle of co-ordinate rotation θ will not be continuous across such a switch between co-ordinate frames, as they represent rotations out of different co-ordinate directions.

The above strategy returns matrices for the rotation and Laplace stretch described in Eqn. (3.23a) for both deformation gradients presented in Eqn. (3.23). The dilemma is remedied. Laplace stretch, as remedied, therefore has an unique physical interpretation.

This above process is the 2D version of the 3D version presented earlier in §2.1. It is easier to understand what is happening in the 2D case, which is why more detail is presented here. It may certainly happen that even when the 3D co-ordinates are re-indexed there may be one or more of the pentagons whose 2D co-ordinates need to be re-indexed, too.

There are three kinematic variables that describe deformation in a planar membrane: elongation ratios a and b and simple shear g . These variables will vary both temporally and spatially whenever Wachspress' shape functions are used, as described above. The fields introduced above are exported from module `membranes` outlined in Appendix F.2.

3.3.6. Thermodynamic Strains and Strain Rates

In terms of the above physical attributes for stretch, i.e., a, b and g , and their reference values, viz., a_0, b_0 and g_0 , one can define a set of strain attributes derived from thermodynamics, specifically [57]

$$\xi := \ln \left(\sqrt{\frac{a}{a_0}} \frac{b}{b_0} \right) \quad d\xi = \frac{1}{2} \left(\frac{da}{a} + \frac{db}{b} \right) \quad (3.28a)$$

$$\varepsilon := \ln \left(\sqrt{\frac{a}{a_0}} \frac{b_0}{b} \right) \quad d\varepsilon = \frac{1}{2} \left(\frac{da}{a} - \frac{db}{b} \right) \quad (3.28b)$$

$$\gamma := g - g_0 \quad d\gamma = dg \quad (3.28c)$$

whose rates are exact differentials, i.e., they are independent of path—a tacit requirement from thermodynamics [58]. Here ξ denotes dilation, ε denotes squeeze, and γ denotes shear.

3.3.6.1. Stretch Rates

The following approximations for stretch rates were derived by Freed & Zamani [39]. From these, the various strain rates listed in Eqn. (3.28) can be established.

A forward difference formula is used to approximate rates in the reference configuration for the various stretch attributes, as obtained from $\dot{\mathcal{U}}_0 = (\mathcal{U}_1 - \mathcal{U}_0)/h + \mathcal{O}(h)$. This produces

$$da_0 = \frac{a_1 - a_0}{h}, \quad db_0 = \frac{b_1 - b_0}{h}, \quad dg_0 = \frac{a_1}{a_0} \left(\frac{g_1 - g_0}{h} \right). \quad (3.29)$$

A backward difference formula $\dot{\mathcal{U}}_1 = (\mathcal{U}_1 - \mathcal{U}_0)/h + \mathcal{O}(h)$ is used to estimate rates for the various stretch attributes at the end of its first integration step, from which it follows that

$$da_1 = \frac{a_1 - a_0}{h}, \quad db_1 = \frac{b_1 - b_0}{h}, \quad dg_1 = \frac{a_0}{a_1} \left(\frac{g_1 - g_0}{h} \right). \quad (3.30)$$

Curiously, there is a distinction in how the shear rates are approximated at the two nodes for this first interval of integration.

Equations (3.29 & 3.30) are first-order approximations for these derivatives. Second-order approximations can be established whenever $n > 0$ provided the stepsize for step $[n, n+1]$ equals the stepsize for step $[n-1, n]$, where state $n=0$ associates with an initial condition. The backward difference formula $\dot{\mathcal{U}}_{n+1} = (3\mathcal{U}_{n+1} - 4\mathcal{U}_n + \mathcal{U}_{n-1})/2h + \mathcal{O}(h^2)$ then produces stretch rates of

$$\begin{aligned} da_{n+1} &= \frac{3a_{n+1} - 4a_n + a_{n-1}}{2h} \\ db_{n+1} &= \frac{3b_{n+1} - 4b_n + b_{n-1}}{2h} \\ dg_{n+1} &= \frac{2a_n}{a_{n+1}} \left(\frac{g_{n+1} - g_n}{h} \right) - \frac{a_{n-1}}{a_{n+1}} \left(\frac{g_{n+1} - g_{n-1}}{2h} \right) \end{aligned} \quad (3.31)$$

which will require a_{n-1} , b_{n-1} and g_{n-1} to be stored in a finite element setting.

3.4. 3D Irregular Dodecahedra

The primary kinematic variables needed to describe the deformation of an irregular dodecahedron used as a model for an alveolar sac are its volume V (see §2.5) and the differential change in volume dV , with the former following from Eq. (2.14) and the latter coming from a suitable finite difference formula. Whenever the material filling an alveolar sac is air (its normal healthy condition), no further breakdown of these kinematics is required.

However, whenever an alveolar sac is filled with fluid (blood, interstitial fluids, plem, etc.) this fluid can be expected to behave solid-like in the face of a passing shock wave. In this situation, non-uniform measures for strain (i.e., shears) can be expected to arise.

3.4.1. Shape Functions for Interpolating an Irregular Tetrahedron

The shape functions associated with the four vertices of a tetrahedron N_i , $i = 1, 2, 3, 4$, that are used in this work are defined as follows

$$N_1 = 1 - \xi - \eta - \zeta, \quad N_2 = \xi, \quad N_3 = \eta, \quad N_4 = \zeta \quad (3.32a)$$

where ξ , η and ζ represent its natural co-ordinates whereby $0 \leq \xi \leq 1$, $0 \leq \eta \leq 1 - \xi$ and $0 \leq \zeta \leq 1 - \xi - \eta$. Gradients of these shape functions are

$$\begin{aligned} N_{1,\xi} &= -1, & N_{1,\eta} &= -1, & N_{1,\zeta} &= -1 \\ N_{2,\xi} &= 1, & N_{2,\eta} &= 0, & N_{2,\zeta} &= 0 \\ N_{3,\xi} &= 0, & N_{3,\eta} &= 1, & N_{3,\zeta} &= 0 \\ N_{4,\xi} &= 0, & N_{4,\eta} &= 0, & N_{4,\zeta} &= 1 \end{aligned} \quad (3.32b)$$

and consequently the deformation gradient will be constant throughout its volume.

3.4.1.1. Deformation Gradient for an Irregular Tetrahedron

The deformation gradient for a volume element is constructed from

$$\mathbf{F}(\xi, \eta, \zeta) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \begin{bmatrix} \partial u / \partial \xi & \partial u / \partial \eta & \partial u / \partial \zeta \\ \partial v / \partial \xi & \partial v / \partial \eta & \partial v / \partial \zeta \\ \partial w / \partial \xi & \partial w / \partial \eta & \partial w / \partial \zeta \end{bmatrix} \begin{bmatrix} \partial x_0 / \partial \xi & \partial x_0 / \partial \eta & \partial x_0 / \partial \zeta \\ \partial y_0 / \partial \xi & \partial y_0 / \partial \eta & \partial y_0 / \partial \zeta \\ \partial z_0 / \partial \xi & \partial z_0 / \partial \eta & \partial z_0 / \partial \zeta \end{bmatrix}^{-1} \quad (3.33)$$

such that, for the four-node tetrahedron considered here, one has

$$\begin{aligned} \begin{bmatrix} \partial u / \partial \xi & \partial u / \partial \eta & \partial u / \partial \zeta \\ \partial v / \partial \xi & \partial v / \partial \eta & \partial v / \partial \zeta \\ \partial w / \partial \xi & \partial w / \partial \eta & \partial w / \partial \zeta \end{bmatrix} &= \begin{bmatrix} \sum_{i=1}^4 N_{i,\xi} u_i & \sum_{i=1}^4 N_{i,\eta} u_i & \sum_{i=1}^4 N_{i,\zeta} u_i \\ \sum_{i=1}^4 N_{i,\xi} v_i & \sum_{i=1}^4 N_{i,\eta} v_i & \sum_{i=1}^4 N_{i,\zeta} v_i \\ \sum_{i=1}^4 N_{i,\xi} w_i & \sum_{i=1}^4 N_{i,\eta} w_i & \sum_{i=1}^4 N_{i,\zeta} w_i \end{bmatrix} \\ &= \begin{bmatrix} u_2 - u_1 & u_3 - u_1 & u_4 - u_1 \\ v_2 - v_1 & v_3 - v_1 & v_4 - v_1 \\ w_2 - w_1 & w_3 - w_1 & w_4 - w_1 \end{bmatrix} \end{aligned} \quad (3.34a)$$

whose nodal displacements $\mathbf{u}_i := \mathbf{x}_i - \mathbf{x}_{0i}$, $i = 1, 2, 3, 4$, have components $\mathbf{u}_i = u_i \vec{\mathbf{E}}_1 + v_i \vec{\mathbf{E}}_2 + w_i \vec{\mathbf{E}}_3$ when evaluated in the co-ordinate frame of a dodecahedron $(\vec{\mathbf{E}}_1, \vec{\mathbf{E}}_2, \vec{\mathbf{E}}_3)$ with $u_i := x_i - x_{0i}$, $v_i := y_i - y_{0i}$ and $w_i := z_i - z_{0i}$, and where

$$\begin{aligned} \begin{bmatrix} \partial x_0 / \partial \xi & \partial x_0 / \partial \eta & \partial x_0 / \partial \zeta \\ \partial y_0 / \partial \xi & \partial y_0 / \partial \eta & \partial y_0 / \partial \zeta \\ \partial z_0 / \partial \xi & \partial z_0 / \partial \eta & \partial z_0 / \partial \zeta \end{bmatrix} &= \begin{bmatrix} \sum_{i=1}^4 N_{i,\xi} x_{0i} & \sum_{i=1}^4 N_{i,\eta} x_{0i} & \sum_{i=1}^4 N_{i,\zeta} x_{0i} \\ \sum_{i=1}^4 N_{i,\xi} y_{0i} & \sum_{i=1}^4 N_{i,\eta} y_{0i} & \sum_{i=1}^4 N_{i,\zeta} y_{0i} \\ \sum_{i=1}^4 N_{i,\xi} z_{0i} & \sum_{i=1}^4 N_{i,\eta} z_{0i} & \sum_{i=1}^4 N_{i,\zeta} z_{0i} \end{bmatrix} \\ &= \begin{bmatrix} x_{02} - x_{01} & x_{03} - x_{01} & x_{04} - x_{01} \\ y_{02} - y_{01} & y_{03} - y_{01} & y_{04} - y_{01} \\ z_{02} - z_{01} & z_{03} - z_{01} & z_{04} - z_{01} \end{bmatrix} \end{aligned} \quad (3.34b)$$

whose initial nodal positions are $\mathbf{x}_{0i} = x_{0i} \vec{\mathbf{E}}_1 + y_{0i} \vec{\mathbf{E}}_2 + z_{0i} \vec{\mathbf{E}}_3$. This matrix is invertible, because the four vertices of the tetrahedron are distinct. The Jacobian matrix is given by

$$\begin{aligned} \mathbf{J} := \begin{bmatrix} \partial x / \partial \xi & \partial x / \partial \eta & \partial x / \partial \zeta \\ \partial y / \partial \xi & \partial y / \partial \eta & \partial y / \partial \zeta \\ \partial z / \partial \xi & \partial z / \partial \eta & \partial z / \partial \zeta \end{bmatrix} &= \begin{bmatrix} \sum_{i=1}^4 N_{i,\xi} x_i & \sum_{i=1}^4 N_{i,\eta} x_i & \sum_{i=1}^4 N_{i,\zeta} x_i \\ \sum_{i=1}^4 N_{i,\xi} y_i & \sum_{i=1}^4 N_{i,\eta} y_i & \sum_{i=1}^4 N_{i,\zeta} y_i \\ \sum_{i=1}^4 N_{i,\xi} z_i & \sum_{i=1}^4 N_{i,\eta} z_i & \sum_{i=1}^4 N_{i,\zeta} z_i \end{bmatrix} \\ &= \begin{bmatrix} x_2 - x_1 & x_3 - x_1 & x_4 - x_1 \\ y_2 - y_1 & y_3 - y_1 & y_4 - y_1 \\ z_2 - z_1 & z_3 - z_1 & z_4 - z_1 \end{bmatrix} \end{aligned} \quad (3.34c)$$

which is used in integrations. Its current nodal positions are $\mathbf{x}_i = x_i \vec{\mathbf{E}}_1 + y_i \vec{\mathbf{E}}_2 + z_i \vec{\mathbf{E}}_3$, $i = 1, 2, 3, 4$. The Jacobian matrix is also invertible, because the four vertices of a tetrahedron are distinct.

3.4.2. QR Factorization of \mathbf{F}

The re-indexed deformation gradient presented in §2.1 has a Gram-Schmidt decomposition that we denote as $\mathbf{F} = \mathcal{R}\mathcal{U}$ wherein $\mathcal{R} = [\vec{\mathbf{g}}_1 \mid \vec{\mathbf{g}}_2 \mid \vec{\mathbf{g}}_3] = \delta_{ij} \vec{\mathbf{g}}_i \otimes \vec{\mathbf{E}}_j = \mathcal{R}_{ij} \vec{\mathbf{E}}_i \otimes \vec{\mathbf{E}}_j$ is a Gram rotation with orthogonal components, and $\mathcal{U} = \mathcal{U}_{ij} \vec{\mathbf{E}}_i \otimes \vec{\mathbf{E}}_j$ is a Laplace stretch [42] with upper-triangular components, so that $\mathbf{F} = \mathcal{F}_{ij} \vec{\mathbf{E}}_i \otimes \vec{\mathbf{E}}_j = \mathcal{R}_{ik} \mathcal{U}_{kj} \vec{\mathbf{E}}_i \otimes \vec{\mathbf{E}}_j$.

The components of Laplace stretch \mathcal{U}_{ij} are readily gotten through a Cholesky factorization of the right Cauchy-Green deformation tensor, here taken to be $\mathbf{C} = \mathcal{C}_{ij} \vec{\mathbf{E}}_i \otimes \vec{\mathbf{E}}_j$ with components $\mathcal{C}_{ij} = \mathcal{F}_{ki} \mathcal{F}_{kj}$ (no eigen analysis is required). Laplace stretch has elements [57]

$$\mathcal{U} = \begin{bmatrix} a & a\gamma & a\beta \\ 0 & b & b\alpha \\ 0 & 0 & c \end{bmatrix} \quad \text{with inverse} \quad \mathcal{U}^{-1} = \begin{bmatrix} 1/a & -\gamma/b & -(\beta - \alpha\gamma)/c \\ 0 & 1/b & -\alpha/c \\ 0 & 0 & 1/c \end{bmatrix} \quad (3.35)$$

with components \mathcal{U}_{ij} being evaluated according to the formulæ [49]

$$\begin{aligned} \mathcal{U}_{11} &= \sqrt{\mathcal{C}_{11}} & \mathcal{U}_{12} &= \mathcal{C}_{12}/\mathcal{U}_{11} & \mathcal{U}_{13} &= \mathcal{C}_{13}/\mathcal{U}_{11} \\ \mathcal{U}_{21} &= 0 & \mathcal{U}_{22} &= \sqrt{\mathcal{C}_{22} - \mathcal{U}_{12}^2} & \mathcal{U}_{23} &= (\mathcal{C}_{23} - \mathcal{U}_{12}\mathcal{U}_{13})/\mathcal{U}_{22} \\ \mathcal{U}_{31} &= 0 & \mathcal{U}_{32} &= 0 & \mathcal{U}_{33} &= \sqrt{\mathcal{C}_{33} - \mathcal{U}_{13}^2 - \mathcal{U}_{23}^2} \end{aligned} \quad (3.36)$$

so that

$$a := \mathcal{U}_{11}, \quad b := \mathcal{U}_{22}, \quad c := \mathcal{U}_{33}, \quad \alpha := \frac{\mathcal{U}_{23}}{\mathcal{U}_{22}}, \quad \beta := \frac{\mathcal{U}_{13}}{\mathcal{U}_{11}}, \quad \gamma := \frac{\mathcal{U}_{12}}{\mathcal{U}_{11}} \quad (3.37)$$

where a , b and c are three, orthogonal, elongation ratios, and where α , β and γ are three, orthogonal, simple shears, with a_0 , b_0 , c_0 , α_0 , β_0 and γ_0 denoting their values in some reference state. The elongations must be positive whereas the shears may be of either sign. Collectively, they constitute a complete set of physical attributes for describing stretch from which constitutive equations can then be constructed.

3.4.3. Thermodynamic Strains and Strain Rates

In terms of the above physical attributes for stretch, one can define a set of strain attributes derived from thermodynamics, specifically [57]

$$\Xi := \ln \left(\sqrt[3]{\frac{a}{a_0} \frac{b}{b_0} \frac{c}{c_0}} \right) \quad d\Xi = \frac{1}{2} \left(\frac{da}{a} + \frac{db}{b} + \frac{dc}{c} \right) \quad (3.38a)$$

$$\varepsilon_1 := \ln \left(\sqrt[3]{\frac{a}{a_0} \frac{b_0}{b}} \right) \quad d\varepsilon_1 = \frac{1}{3} \left(\frac{da}{a} - \frac{db}{b} \right) \quad (3.38b)$$

$$\varepsilon_2 := \ln \left(\sqrt[3]{\frac{b}{b_0} \frac{c_0}{c}} \right) \quad d\varepsilon_2 = \frac{1}{3} \left(\frac{db}{b} - \frac{dc}{c} \right) \quad (3.38c)$$

$$\gamma_1 := \alpha - \alpha_0 \quad d\gamma_1 = d\alpha \quad (3.38d)$$

$$\gamma_2 := \beta - \beta_0 \quad d\gamma_2 = d\beta \quad (3.38e)$$

$$\gamma_3 := \gamma - \gamma_0 \quad d\gamma_3 = d\gamma \quad (3.38f)$$

whose rates are exact differentials, i.e., they are independent of path—a tacit requirement from thermodynamics [58]. Here Ξ represents dilatation, ε_1 is a squeeze in the 12 plane, and ε_2 is a squeeze in the 23-plane, while γ_1 is a shear in the 23 plane, γ_2 is a shear in the 13 plane, and γ_3 is a shear in the 12 plane, which are three, orthogonal, simple shearing motions. There is a third squeeze, too, viz., $\varepsilon_3 = -\varepsilon_1 - \varepsilon_2$, but it is not an independent descriptor of strain.

3.4.3.1. Stretch Rates

The following approximations for stretch rates were derived by Freed & Zamani [39]. From these, the various strain rates listed in Eqn. (3.38) can be established.

A forward difference formula is used to approximate rates in the reference configuration for the various stretch attributes, as obtained from $\dot{\mathcal{U}}_0 = (\mathcal{U}_1 - \mathcal{U}_0)/h + \mathcal{O}(h)$. This produces

$$\begin{aligned} da_0 &= \frac{a_1 - a_0}{h} & d\alpha_0 &= \frac{b_1}{b_0} \left(\frac{\alpha_1 - \alpha_0}{h} \right) \\ db_0 &= \frac{b_1 - b_0}{h} & d\beta_0 &= \frac{a_1}{a_0} \left(\frac{\beta_1 - \beta_0}{h} \right) \\ dc_0 &= \frac{c_1 - c_0}{h} & d\gamma_0 &\approx \frac{a_1}{a_0} \left(\frac{\gamma_1 - \gamma_0}{h} \right). \end{aligned} \quad (3.39)$$

A backward difference formula $\dot{\mathcal{U}}_1 = (\mathcal{U}_1 - \mathcal{U}_0)/h + \mathcal{O}(h)$ is used to estimate rates for the various stretch attributes at the end of its first integration step, from which it follows that

$$\begin{aligned} da_1 &= \frac{a_1 - a_0}{h} & d\alpha_1 &= \frac{b_0}{b_1} \left(\frac{\alpha_1 - \alpha_0}{h} \right) \\ db_1 &= \frac{b_1 - b_0}{h} & d\beta_1 &= \frac{a_0}{a_1} \left(\frac{\beta_1 - \beta_0}{h} \right) \\ dc_1 &= \frac{c_1 - c_0}{h} & d\gamma_1 &= \frac{a_0}{a_1} \left(\frac{\gamma_1 - \gamma_0}{h} \right). \end{aligned} \quad (3.40)$$

Curiously, there is a distinction in how the shear rates are approximated at the two nodes for this first interval of integration.

Equations (3.39 & 3.40) are first-order approximations for these derivatives. Second-order approximations can be established whenever $n > 0$ provided the stepsize for step $[n, n+1]$ equals the stepsize for step $[n-1, n]$, where state $n=0$ associates with an initial condition. The backward difference formula $\dot{\mathcal{U}}_{n+1} = (3\mathcal{U}_{n+1} - 4\mathcal{U}_n + \mathcal{U}_{n-1})/2h + \mathcal{O}(h^2)$ produces differential stretch rates of

$$\begin{aligned} da_{n+1} &= \frac{3a_{n+1} - 4a_n + a_{n-1}}{2h} \\ db_{n+1} &= \frac{3b_{n+1} - 4b_n + b_{n-1}}{2h} \\ dc_{n+1} &= \frac{3c_{n+1} - 4c_n + c_{n-1}}{2h} \\ d\alpha_{n+1} &= \frac{2b_n}{b_{n+1}} \left(\frac{\alpha_{n+1} - \alpha_n}{h} \right) - \frac{b_{n-1}}{b_{n+1}} \left(\frac{\alpha_{n+1} - \alpha_{n-1}}{2h} \right) \\ d\beta_{n+1} &= \frac{2a_n}{a_{n+1}} \left(\frac{\beta_{n+1} - \beta_n}{h} \right) - \frac{a_{n-1}}{a_{n+1}} \left(\frac{\beta_{n+1} - \beta_{n-1}}{2h} \right) \\ d\gamma_{n+1} &= \frac{2a_n}{a_{n+1}} \left(\frac{\gamma_{n+1} - \gamma_n}{h} \right) - \frac{a_{n-1}}{a_{n+1}} \left(\frac{\gamma_{n+1} - \gamma_{n-1}}{2h} \right) \end{aligned} \quad (3.41)$$

which require data to be stored for the previous state associated with step $n-1$.

3.5. Code Verification: Kinematics

The thermodynamic conjugate pairs of Freed *et al.* [51, 52, 57] result in the following geometric/thermodynamic strain measures for our dodecahedral model: for 1D rods, an axial strain $e = \ln(L/L_0)$; for 2D membranes, a dilation $\xi = \ln \sqrt{ab/a_0 b_0} = \ln \sqrt{A/A_0}$, a squeeze (or pure shear) $\varepsilon = \ln \sqrt{ab_0/a_0 b} = \ln \sqrt{\Gamma/\Gamma_0}$, and a (simple) shear $\gamma = g - g_0$; and for 3D dodecahedra, a dilatation $\Xi = \ln \sqrt[3]{V/V_0}$ and, for those cases where the medium within an alveolar sac can support non-uniform stresses, two squeezes $\varepsilon_1 = \ln \sqrt[3]{ab_0/a_0 b}$ and $\varepsilon_2 = \ln \sqrt[3]{bc_0/b_0 c}$ plus three shears $\gamma_1 = \alpha - \alpha_0$, $\gamma_2 = \beta - \beta_0$ and $\gamma_3 = \gamma - \gamma_0$.

3.5.1. Isotropic Motions

Imposing the uniform far-field motion of a volumetric expansion onto our dodecahedral model results in a dodecahedral dilatation ($\Xi := \ln \sqrt[3]{V/V_0}$) that equals its pentagonal dilation ($\xi := \ln \sqrt{A/A_0}$) that equals its chordal strain ($e := \ln(L/L_0)$). These three strain measures follow from the 3-mode thermodynamic theory of Freed *et al.* [51, 52]. Other choices for strain measures do not result in one-to-one relationships when exposed to an isotropic motion like those observed here. This is a particularly useful result in that it establishes a meaningful scaling in terms of strains between the three dimensions, cf. Fig. 3.5. It also provides for a verification of the numerical implementation of our dodecahedral model.

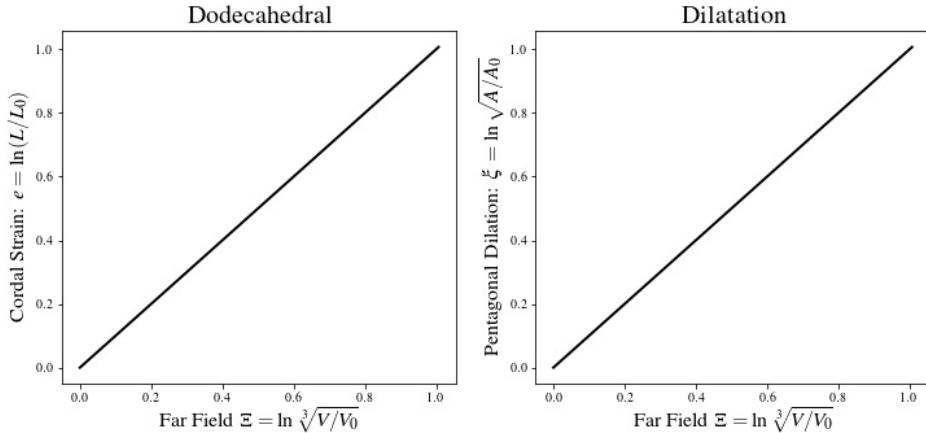


Figure 3.5: Response of a dodecahedron exposed to an isotropic motion of dilatation. The abscissa is the control variable and the ordinates are response variables. The right graphic plots the areal response of the pentagons $\xi = \ln \sqrt{A/A_0}$, while the left graphic plots the axial response of the chords $e = \ln(L/L_0)$. Both are plotted against the volumetric response of the dodecahedron $\Xi = \ln \sqrt[3]{V/V_0}$. Here V denotes dodecahedral volume, A denotes pentagonal area, and L denotes chordal length, all being evaluated in the current state, whose reference values are V_0 , A_0 and L_0 .

3.5.1.1. Geometric vs. Thermodynamic Strains

There are two types of strain measures that one can use to quantify deformation within a pentagon of a dodecahedron: geometric and thermodynamic. For the uniform far-field motion of volumetric expansion, only the thermodynamic strain known as dilation, i.e., $\xi = \ln \sqrt{ab/a_0 b_0}$, varies with the motion, and its response equals that of the geometric strain $\ln \sqrt{A/A_0}$, see Fig. 3.6. Also present in this graph is an observation that the thermodynamic strains for squeeze ε and shear γ do not contribute under motions of pure dilatation, as expected. This further verifies the numerical implementation of our dodecahedral model.

To put this into perspective, we compare with studies done by multiple investigators where ratios of alveolar surface area, viz., A/A_0 , have been measured in rat, rabbit, guinea pig, and cat, cf. Roan & Waters [17, Table 1]. These experiments considered ranges that went as low as 25% and as high as 100% of total lung capacity. Taking statistics of their tabulation produced results of: $A/A_0 = 1.47 \pm 0.44$ during inflation and $A/A_0 = 1.18 \pm 0.14$ during deflation, which correspond to a $\xi = \ln \sqrt{A/A_0} = 0.19 \pm 0.18$ for inflation and a $\xi = \ln \sqrt{A/A_0} = 0.08 \pm 0.07$ for deflation. These areal strains values coincide with the chordal strains of $e = \ln(L/L_0) = 0.13$ measured *in vivo* around the periphery of an alveolus in rat lung, as reported by Perlman & Bhattachary [59]. Our kinematics have been verified well past these physiologic ranges, viz., for dilatations up to 100% logarithmic strain.

3.5.2. Isochoric Motions

The motions of pure and simple shears are volume preserving. Imposing these shears as far-field motions onto our dodecahedral model produced the results displayed in Fig. 3.7. For a simple shear, the numerical model is in error by about machine precision, i.e., $\epsilon_m \approx$

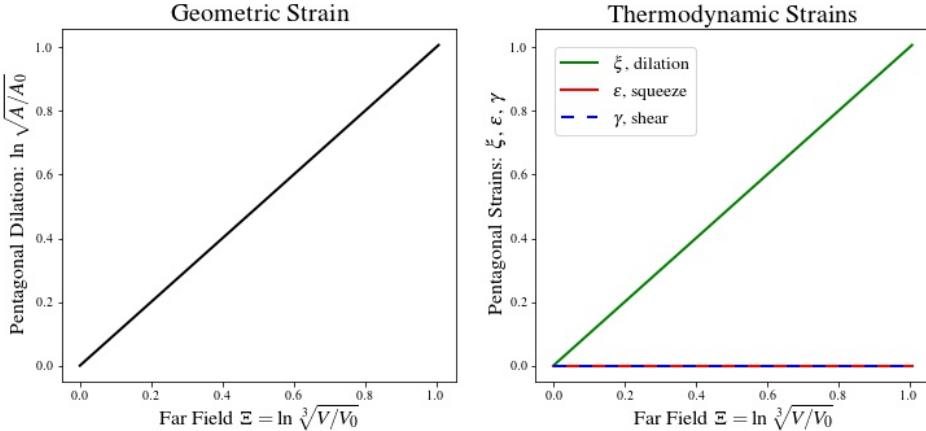


Figure 3.6: Response of a dodecahedron exposed to a far-field isotropic motion of dilatation. The abscissa is the control variable and the ordinates are response variables. The right graphic plots the three thermodynamic strains, as they apply to a pentagon, while the left graphic plots the geometric strain of a pentagon.

2.2×10^{-16} , for strains up to 100%, while for pure shear (a special case of squeeze in 3D) the model is in error by about machine precision for strains up to of about 60%, after which the error further increases, up to about $10\epsilon_m$ at strains around 100%. This further verifies the numerical implementation of our dodecahedral model.

3.5.2.1. Geometric Strains

How the thirty chords and the twelve irregular pentagons deform under far-field motions of pure shear is displayed in Fig. 3.8. Figure 3.7 demonstrates that the overall response of a dodecahedron is isochoric during pure shear. Regardless, Fig. 3.8 demonstrates that the individual chordal and pentagonal constituents deform in a non-homogeneous manner, where the strains have been calculated as geometric changes in dodecahedral shape. This result agrees with *in vivo* observations made by Perlman & Bhattacharya [59] where confocal microscopy was used to image a breathing rat lung.

For the dodecahedral chords, there are six independent responses for motions of pure shear: two chords each for three of these lines, and eight chords each for the remaining three curves present in the left images of Fig. 3.8. For pentagons, there are three independent responses with four pentagons responding according to each curve shown in the right images. Although different chords and pentagons deform differently when sheared in different directions, their collective responses are the same regardless of the far-field direction being sheared. Consequently, the local geometric response of a dodecahedron is isotropic under the far-field motions of pure shear.

How the thirty chords and the twelve irregular pentagons deform under far-field motions of simple shear is displayed in Fig. 3.9. Figure 3.7 demonstrates that the overall response of a dodecahedron is isochoric during a far-field simple shear. Figure 3.9 demonstrates that the individual chordal and pentagonal constituents deform in a non-homogeneous manner during simple shears, like they do for pure shears. However, unlike pure shears whose collective

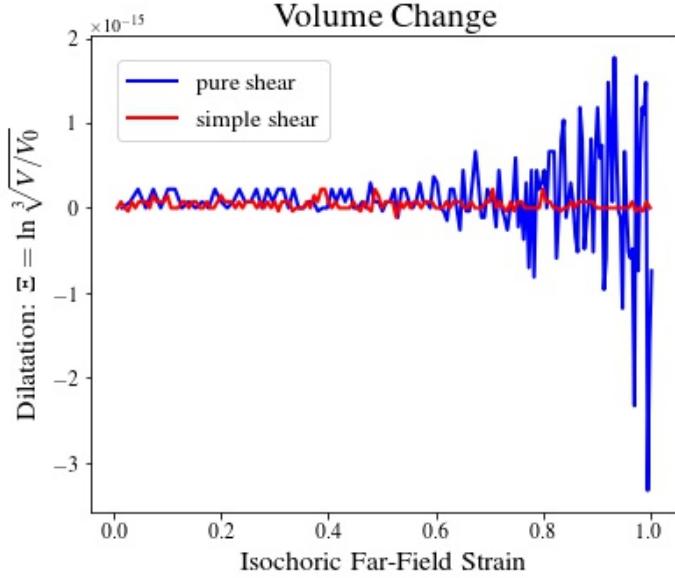


Figure 3.7: Response of a dodecahedron exposed to far-field motions of pure and simple shears. Note that the ordinate is $\times 10^{-15}$ and machine precision is $\sim 2.2 \times 10^{-16}$.

chordal and pentagonal responses remain isotropic, here they diverge from isotropy under motions of simple shear. Simple shears in the 12 and 23 planes have the same collective response; whereas, simple shear in the 13 plane has a slightly different response.

Figures 3.5–3.9 establish that a dodecahedron is (nearly, but not completely) isotropic in its kinematic response, as measured by the geometric strains $e = \ln(L/L_0)$, $\xi = \ln\sqrt{A/A_0}$ and $\Xi = \ln\sqrt[3]{V/V_0}$. Furthermore, even though a far-field deformation is homogeneous, in accordance with Conjecture 1, the local deformations within the individual constituents of an alveolus will typically be heterogeneous, which agrees with imaging data [59].

3.5.2.2. Thermodynamic Strains

Addressing the septal response, modeled here as a set of twelve irregular pentagons per alveolus, we desire to come to a determination regarding how to best model the deformation occurring within these alveolar septa. In the section above we investigated the geometric response of alveolar septa via the strain measure $\ln\sqrt{A/A_0}$, which quantifies dilation.

The thermodynamic strains arising from a Gram-Schmidt factorization of the deformation gradient put forward in §3.3.5 specify three strain measures pertinent to a membrane: dilation $\xi = \ln\sqrt{ab/a_0 b_0}$, squeeze $\varepsilon = \ln\sqrt{ab_0/a_0 b}$ and shear $\gamma = g - g_0$, where elongations a and b and magnitude of shear g are illustrated in Fig. 3.2. Of these, dilation is an uniform response, while squeeze and shear describe non-uniform responses. To acquire them requires knowing the deformation gradient.

The curves in Figs. 3.8 & 3.9 were obtained from geometric measures for chordal strain $\ln(L/L_0)$ and areal dilation $\ln\sqrt{A/A_0}$. They were computed under separate conditions of pure and simple far-field shears. The curves in Figs. 3.10 & 3.11 were obtained from thermo-

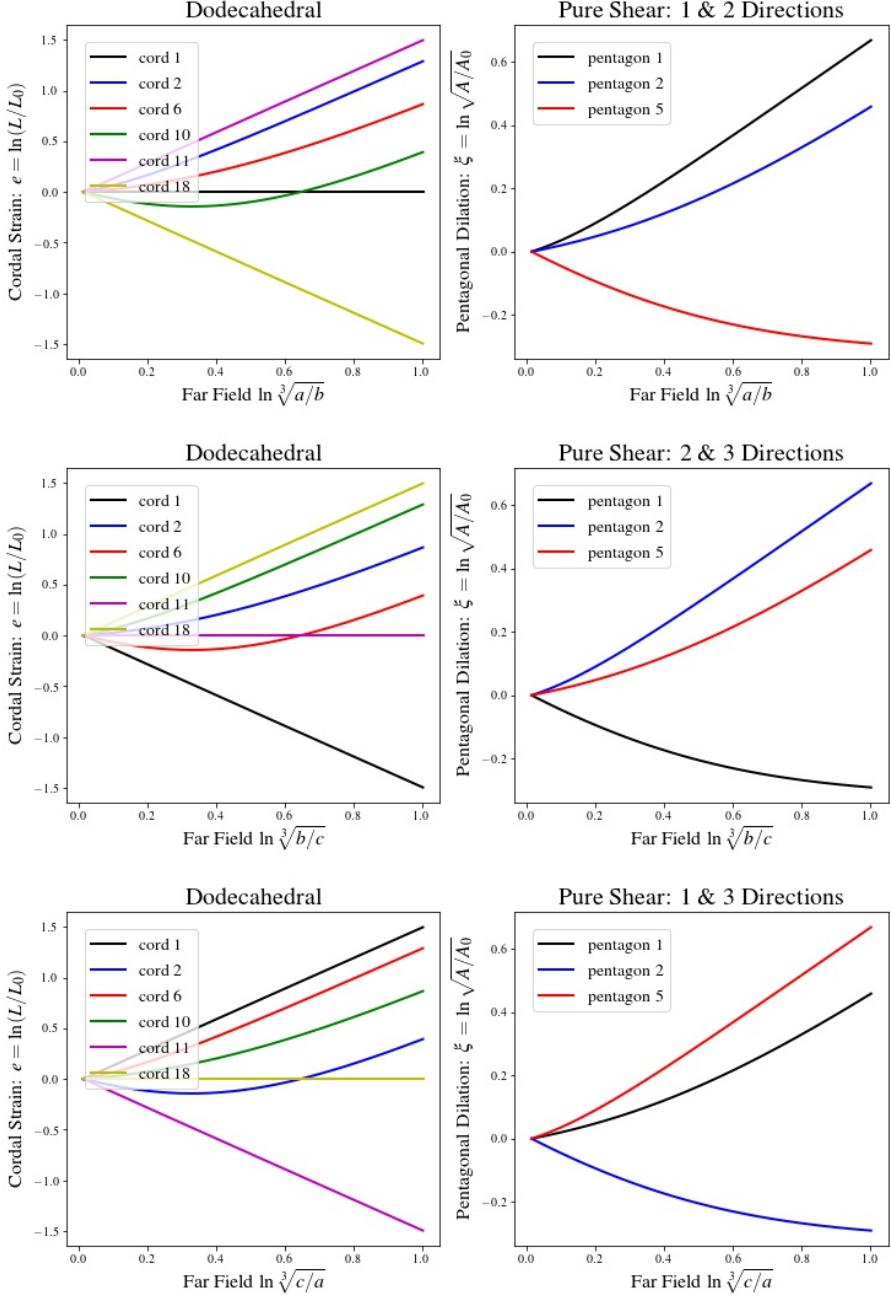


Figure 3.8: Response of a dodecahedron exposed to far-field pure-shear motions in the sense of Treloar [60]: $a = \ell$, $b = 1/\ell$ and $c = 1$ in the top images; $a = 1$, $b = \ell$ and $c = 1/\ell$ in the middle images; and $a = 1/\ell$, $b = 1$ and $c = \ell$ in the bottom images, with ℓ denoting an elongation of extrusion. In all six graphic images, the relevant (controlled) motion of the far-field pure shear is plotted along the abscissa. In each image pair, the right graphic presents pentagonal dilations, while the left graphic presents chordal elongations. Only unique responses are plotted; repetitions are not.

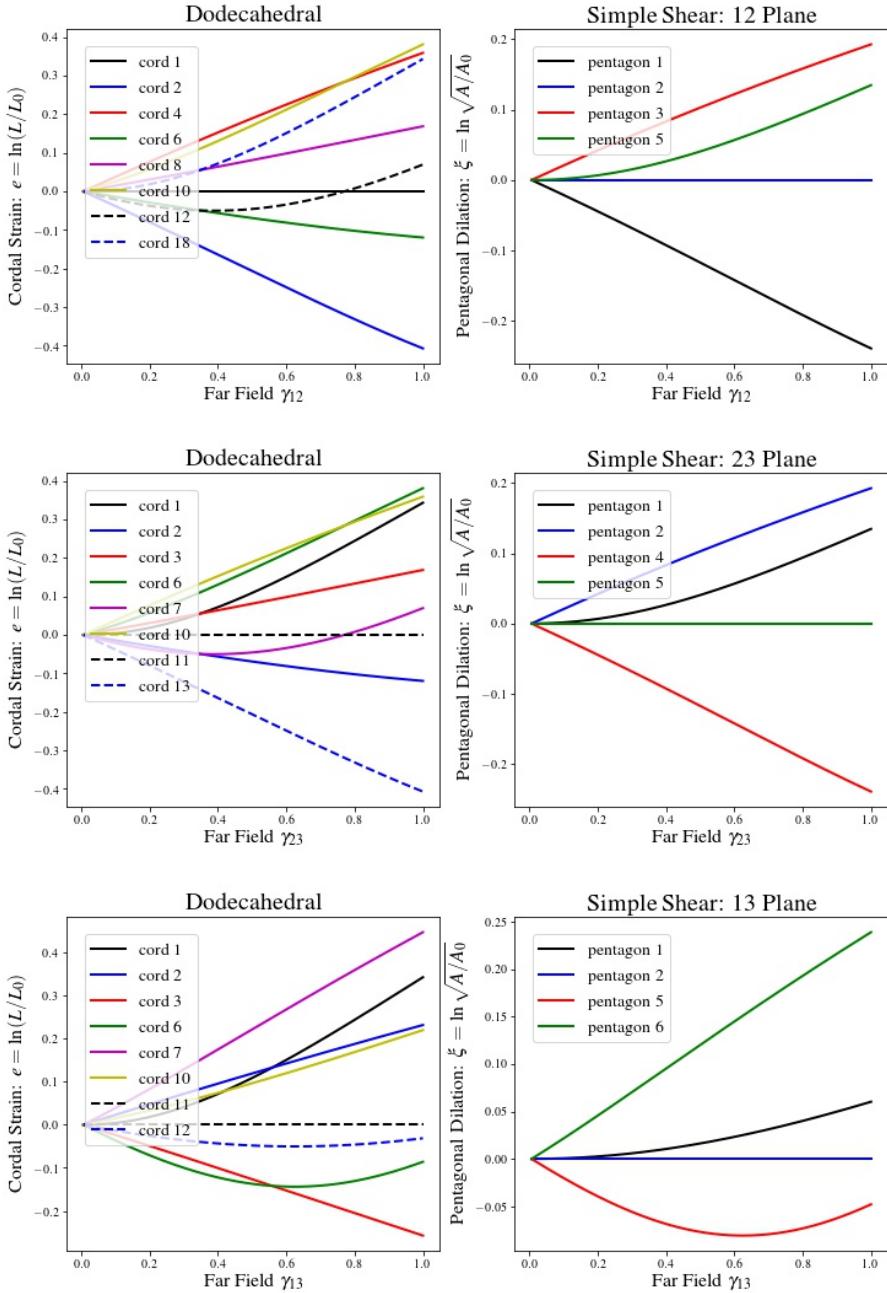


Figure 3.9: Response of a dodecahedron exposed to far-field simple-shear motions. In all six graphic images, the relevant (controlled) motion of simple shear is plotted along the abscissa. In each image pair, the right graphic presents pentagonal dilations, while the left graphic presents chordal elongations. Only unique responses are plotted; repetitions are not.

dynamic measures for membrane strain under the same far-field deformations. The strains of dilation ξ , squeeze ε , and shear γ were computed in accordance with §3.3.5 using deformation gradients gotten from the pentagonal shape functions of Wachspress [43] discussed in §3.3.1.⁵

Figures 3.8–3.11 allow us to conclude that if septal dilation were the only mode of planar deformation thought to cause a mechanical response, then knowledge of the geometric strain $\xi = \ln \sqrt{A/A_0}$ would be adequate; there would be no need to introduce a separate finite-element discretization of the septal planes for acquiring their deformation gradients. However, if the non-uniform responses of squeeze ε and shear γ are thought to contribute to the overall mechanical response of these membranes, then the shape functions of Wachspress [43, 44] ought to be used for acquiring the deformation gradient within a septal plane. We found, but do not present figures to support this observation, that constant-strain triangles are not accurate enough for our application. Strains derived from Wachspress shape functions are inhomogeneous; consequently, the deformation gradient will need to be evaluated at each Gauss point of integration within a pentagon, cf. §5.2.

3.5.3. Co-ordinate Pivoting

The pivoting strategy of §3.3.5.3 used to address the physical dilemma of §3.3.5.2 did not engage often during our assessment of the code, but it did arise at least twice with effects illustrated in Figs. 3.12 & 3.13. Here one can see that there is a clear effect on the shear response within four pentagonal planes; however, no change is observed to have occurred in either the dilation or squeeze responses, as expected. It is not always possible to know when or where a co-ordinate relabeling ought to occur; consequently, the algorithm put forward in §3.3.5.3 is deemed necessary.

3.5.4. Compatible Membrane Deformations

For a deformation to be compatible, and therefore integrable, the curl of its deformation gradient must vanish, viz., $\text{curl}(\mathbf{F}) = \mathbf{0}$ [48]. Equation (3.15) provides constraint equations for the compatibility of planar motions, e.g., septal planes of an alveolus. Here we test to make sure that these conditions are satisfied within the pentagonal planes of our alveolar dodecahedron, assuming that the shape functions of Wachspress apply.

Figure 3.14 presents the compatibility response at the centroid of a typical pentagonal plane during the uniform expansion of a regular dodecahedron out to 100% strain. Theoretically, all four derivatives should be zero for this motion. Actually, their values are on the order of machine precision. Most importantly, whenever they are not zero, they lie along the 45° diagonal, thereby verifying compatibility in the case of a dilatation.

Similarly, Figs. 3.15 & 3.16 present typical responses for testing compatibility during far-field pure shear (Fig. 3.15) and simple shear (Fig. 3.16) deformations. In both cases, one of the four pentagons around the girth of the dodecahedron (viz., #5) has been selected, as both modes of deformation are activated in this pentagon. In both cases, errors are typically

⁵Five constant-strain triangles were also used to quantify the deformation gradient for each pentagonal surface at its centroid—the common vertex to all five triangles. This approach provided accurate descriptions for uniform strain, i.e., dilation ξ , but not for the two non-uniform strains, viz., squeeze ε and shear γ .

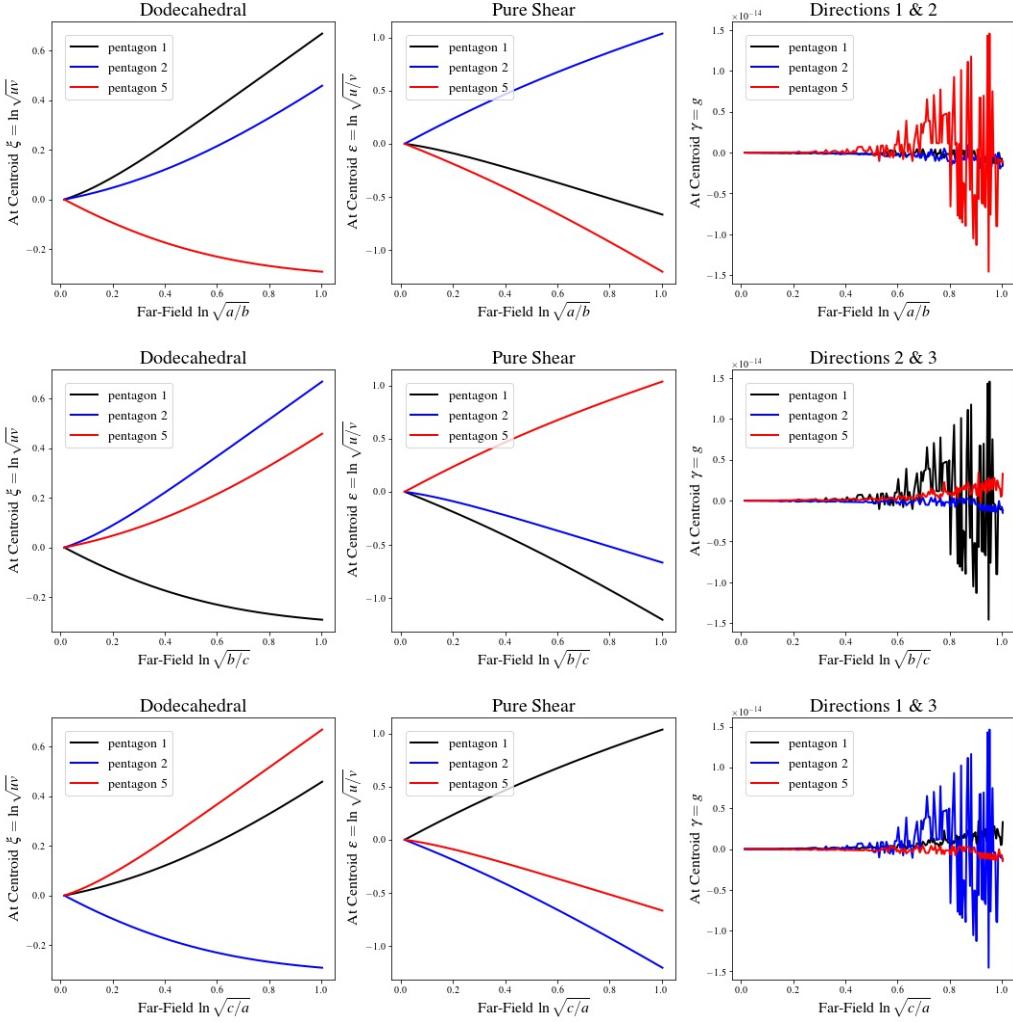


Figure 3.10: Same boundary conditions as in Fig. 3.8. Pentagonal areas were used to compute dilation in Fig. 3.8. The shape functions of Wachspress were used to compute dilation here. The uniform response in the right column of Fig. 3.8 and in the left column above are the same, providing additional assurance that the code has been correctly implemented. The squeeze response shown in the center column is the same for all three orientations of far-field pure shear, i.e., this response is isotropic. The right column has ordinates scaled by 10^{-14} implicating that there is no simple shear response occurring within any pentagonal surface of the dodecahedron whenever it is subjected to a far-field motion of pure shear.

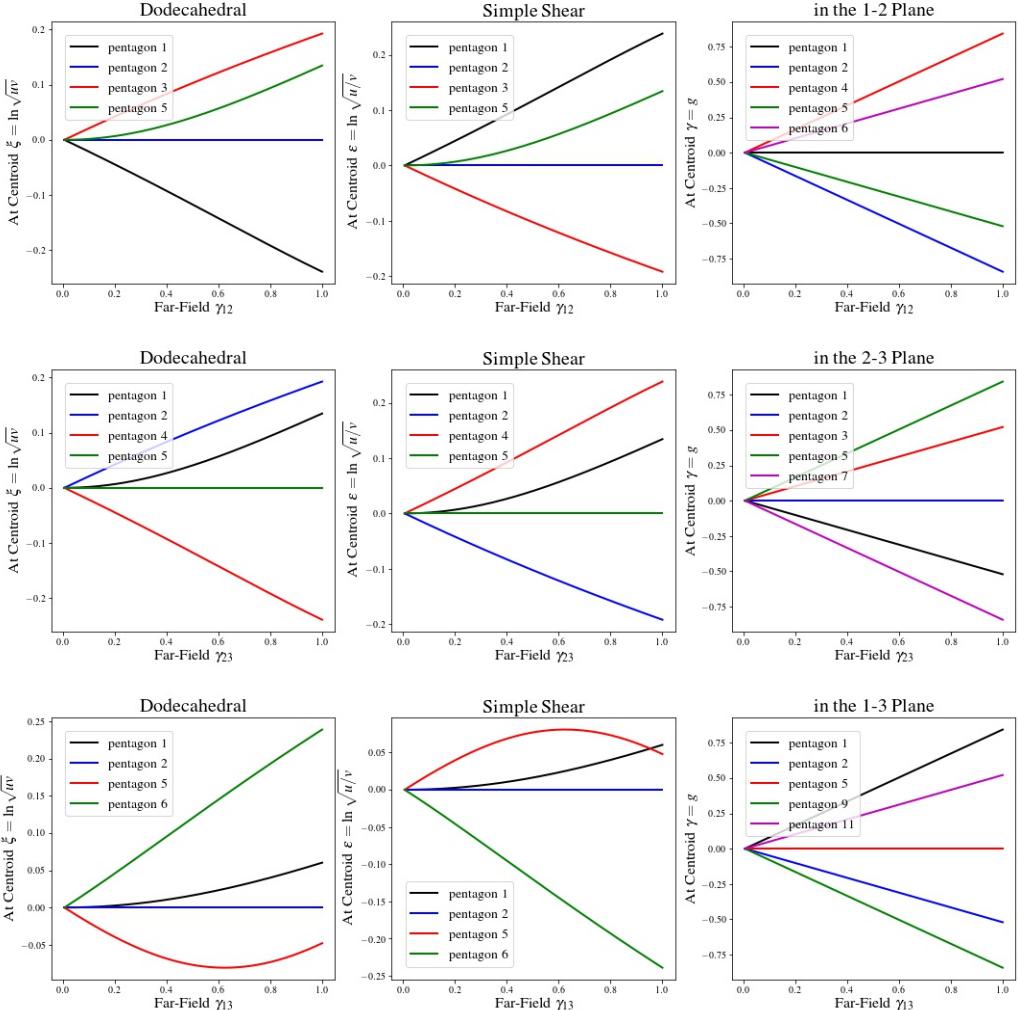


Figure 3.11: Same boundary conditions as in Fig. 3.9. Pentagonal areas were used to compute dilation in Fig. 3.9. The shape functions of Wachspress were used to compute dilation here. The uniform response in the right column of Fig. 3.9 and in the left column above are the same, providing additional assurance that the code has been correctly implemented. Like the dilational responses of the left column, the squeeze responses of the center column are the same in the 1-2 and 2-3 planes, but differ in the 1-3 plane. In all cases, the simple shear response of any pentagonal plane is proportional to that of the far-field shear imposed, further substantiating the code's implementation. The shear response of the septal membranes is isotropic.

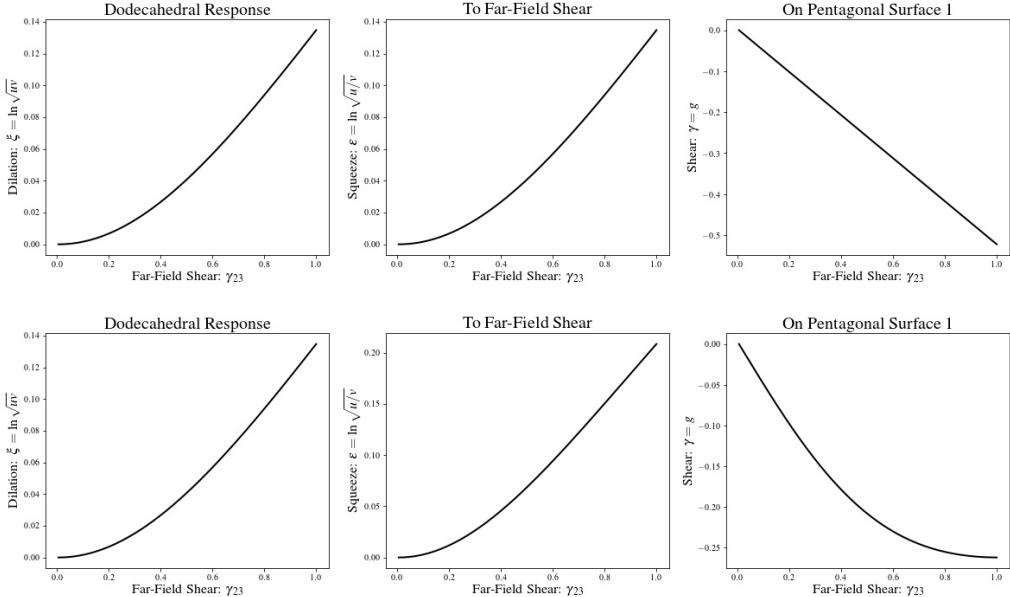


Figure 3.12: A far-field shear of γ_{23} is imposed on the dodecahedron. Pentagons 1 and 8 exhibit the plotted response. The top set of figures result whenever the pivoting strategy of §3.3.5.3 is used, while the bottom set of figures result whenever no pivoting strategy is employed. The dilation (left graphs) and squeeze (center graphs) responses are not effected by pivoting, only shear (right graphs) is effected. Pivoting maintains a linear shear response under a far-field shearing of the dodecahedron, as desired.

less than ten times machine precision, thereby verifying compatibility in the cases of squeeze and shear.

This collective set of graphs, Figs. 3.14–3.16, investigate the constraint of compatibility in terms of the three fundamental modes of deformation: dilatation, squeeze and shear. These figures verify that the constraint of compatibility is satisfied when using the pentagonal shape functions of Wachspress [43, 44] in our dodecahedral model, as errors are typically less than ten times machine precision. This has been verified out to deformations that are at least three times those of their normal physiologic range.

Our kinematic analysis of a dodecaheron has been verified theoretically and numerically.

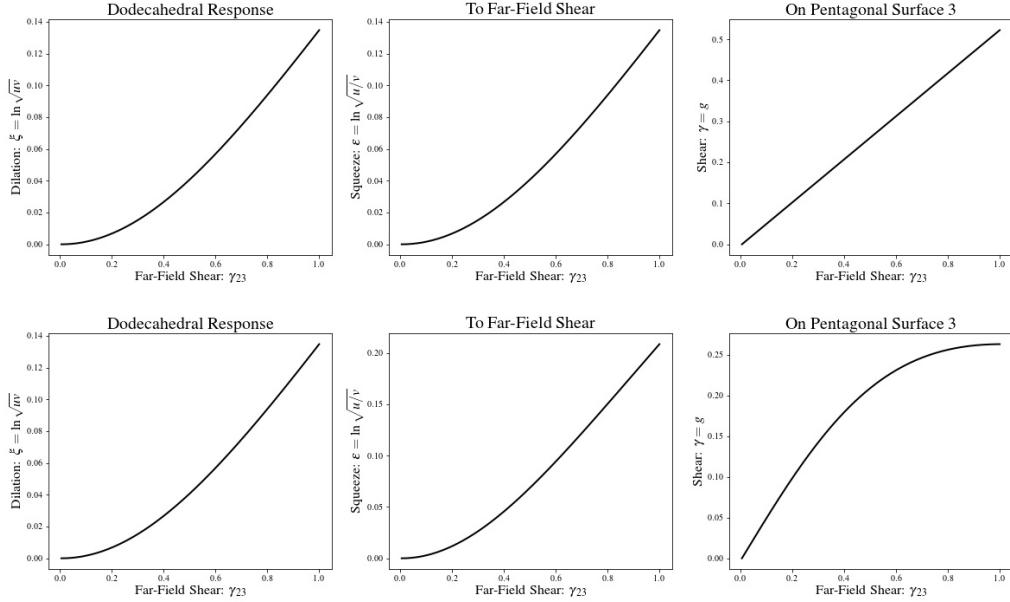


Figure 3.13: A far-field shear of γ_{23} is imposed on the dodecahedron. Pentagons 3 and 10 exhibit the plotted response. The top set of figures result whenever the pivoting strategy of §3.3.5.3 is used, while the bottom set of figures result whenever no pivoting strategy is employed. The dilation (left graphs) and squeeze (center graphs) responses are not effected by pivoting, only shear (right graphs) is effected. Pivoting maintains a linear shear response under a far-field shearing of the dodecahedron, as desired.

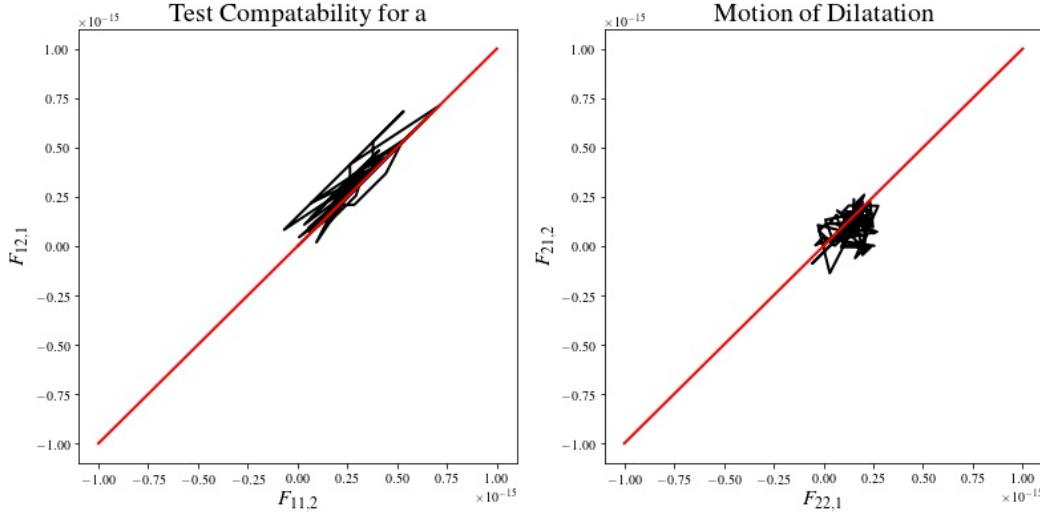


Figure 3.14: Planar compatibility requires $F_{11,2} = F_{12,1}$ and $F_{22,1} = F_{21,2}$ where the left-hand sides are plotted as the abscissæ and the right-hand sides are plotted as the ordinates. For compatibility, the response ought to lie along the 45° diagonal, which is drawn in red over the range of $\pm 10^{-15}$ where machine precision is about 2.2×10^{-16} . Here the motion is one of uniform dilatation out to 100% strain.

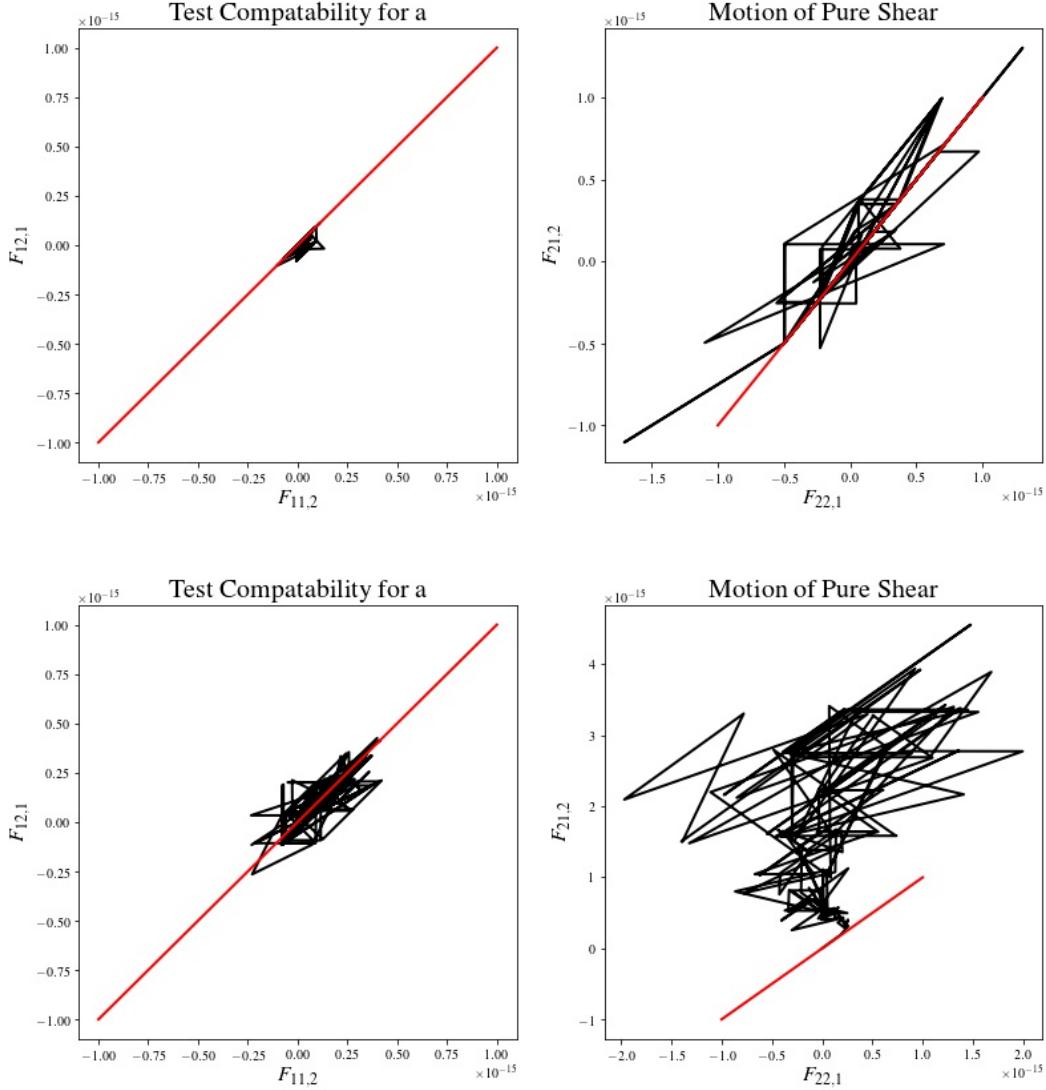


Figure 3.15: Planar compatibility requires $F_{11,2} = F_{12,1}$ and $F_{22,1} = F_{21,2}$ where the left-hand sides are plotted as the abscissæ and the right-hand sides are plotted as the ordinates. For compatibility, the response ought to lie along the 45° diagonal, which is drawn in red over the range of $\pm 10^{-15}$ where machine precision is about 2.2×10^{-16} . Here the motion is one of pure shear out to 100% strain with elongation occurring in the 1-direction, contraction occurring in the 2 direction, while the 3-direction is held fixed. These results pertain to pentagon 5: nodes 15, 5, 12, 11, 1, cf. Fig. 2.1 and Table 2.3. The top row of figures is the best response (at Gauss point 7, cf. Fig. 5.1) while the bottom row of figures is the worst response (at Gauss point 5).

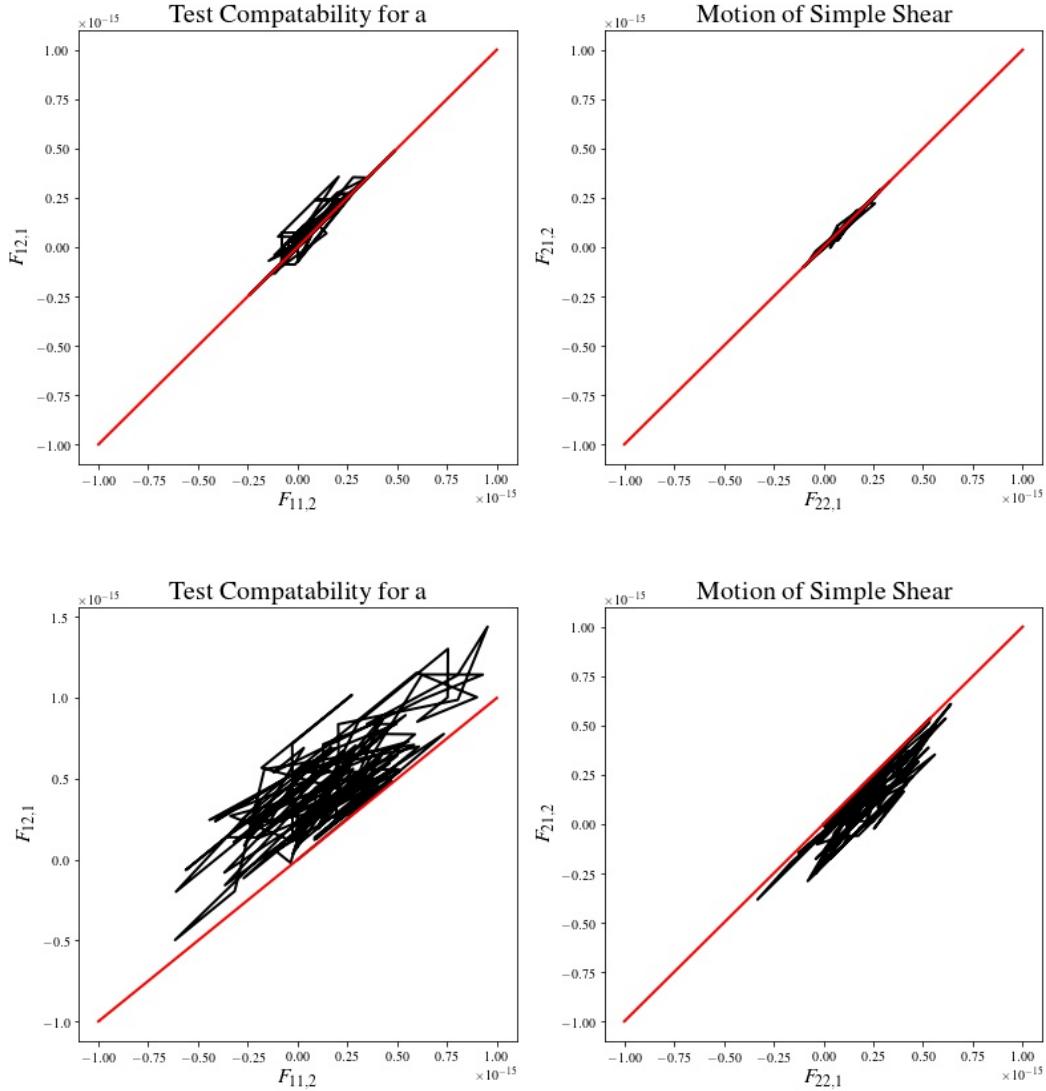


Figure 3.16: Planar compatibility requires $F_{11,2} = F_{12,1}$ and $F_{22,1} = F_{21,2}$ where the left-hand sides are plotted as the abscissæ and the right-hand sides are plotted as the ordinates. For compatibility, the response ought to lie along the 45° diagonal, which is drawn in red over the range of $\pm 10^{-15}$ where machine precision is about 2.2×10^{-16} . Here the motion is one of simple shear out to 100% strain, shearing along 1-2 planes in the 1-direction. These results pertain to pentagon 5: nodes 15, 5, 12, 11, 1, cf. Fig. 2.1 and Table 2.3. The top row of figures is the best response (at Gauss point 7, cf. Fig. 5.1) while the bottom row of figures is the worst response (at Gauss point 5).

Part 4

Constitutive Theory

Roan & Waters [17] and Suki *et al.* [61, 62] have both written extensive review articles on the mechanics of parenchyma, have provided detailed information about the structural constituents of alveoli, and have discussed their influence on the overall mechanical response of parenchyma. Of particular relevance, from a mechanics perspective, are the constituent building blocks of alveolar tissue: collagen (types I and III, predominantly), elastin, proteoglycans and other proteins, surfactant and cells (epithelial and endothelial, predominantly). These constituents are assembled in such a manner so as to produce a variety of alveolar sub-structures that are essentially 1D (alveolar chords), 2D (alveolar septa) and 3D (alveolar sacs) in their geometric construction. Birzle *et al.* [63] have performed a set of experiments on rat parenchyma in an effort to delineate the separate effects of elastin, collagen and the ground substance (everything else) on the collective mechanical response of these tissues.

A dodecahedron is used here as a geometric model for an alveolus [22], cf. Figs. 1.4 & 2.1. It is comprised of: thirty 1D rods that represent alveolar chords, twelve 2D membranes that represent alveolar septa, considered here to be pentagonal in shape, and one 3D cavity filled with air (or fluid in the case of a contusion caused by injury or an edema caused by disease), considered here to be dodecahedral in shape. The thermoelastic constitutive equations presented in this chapter for spatial chords and membranes are derived in Appendix A. Elastic behavior is sufficient for our intended application of studying alveoli when being subjected to traveling waves.

We recall from our kinematic study of a dodecahedron that the geometric strains of $e := \ln(L/L_0)$ for the elongation of septal chords, $\xi := \ln \sqrt{A/A_0}$ for the dilation of septal membranes, and $\Xi := \ln \sqrt[3]{V/V_0}$ for the dilatation of alveolar volume are equivalent to one another under motions of uniform compression/expansion. These three, geometric, strain measures also exist as thermodynamic strains, each associating with a distinct and unique conjugate stress.

Constitutive equations are a derived consequence from physical laws governing thermodynamic processes. Here we derive constitutive equations applicable for 1D thermoelastic fibers (alveolar chords), 2D thermoelastic membranes (alveolar septa), and 3D thermoelastic volumes (alveolar sacs). In §4.1, we assume that the motions are uniform in their spatial dimension. Later, in §4.2 & §4.3, the non-uniform motions of squeeze and shear are included into our thermodynamic framework for membranes and volumes. Section 4.4 pulls these results together, sufficient for the intended purpose of modeling the three structural facets that comprise an alveolous. Specifically, all geometric entities (alveolar chords, alveolar septa, and alveolar sacs) are now described in terms of stresses (dyne/cm^2) instead of their intensive thermodynamic forces (force, surface tension, and stress). This is done to facilitate implementation of these models into code, and to facilitate interpretations of their results by engineers and scientists. The chapter closes with a discussion of their implementation into finite elements in §4.5 and a set of examples created to verify our code in §4.6.

4.1. Green Thermoelastic Solids Subjected to Uniform Motions in 1D, 2D & 3D

Combining the First and Second Laws of Thermodynamics governing uniform, reversible, adiabatic processes results in the following three formulæ, one per dimension; they are

$$\text{In 1 Dimension: } dU = \theta d\eta + \frac{1}{\rho_{1D}} F dL/L \quad (4.1a)$$

$$\text{In 2 Dimensions: } dU = \theta d\eta + \frac{1}{\rho_{2D}} T dA/A \quad (4.1b)$$

$$\text{In 3 Dimensions: } dU = \theta d\eta - \frac{1}{\rho_{3D}} P dV/V \quad (4.1c)$$

wherein U is an internal energy density (erg/gr = dyne.cm/gr), which is a function of state, θ is a temperature in Kelvin ($273 + {}^\circ\text{C}$), η is an entropy density (erg/gr.K), L is a length of line (cm), A is an area of surface (cm^2), V is a volume of space (cm^3), F is a force (dyne), T is a surface tension (dyne/cm), and P is a pressure (dyne/ cm^2 = barye), whereas the mass densities ρ_{1D} (gr/cm), ρ_{2D} (gr/ cm^2) and ρ_{3D} (gr/ cm^3) associate with a reference state of per unit length, or per unit area, or per unit volume, as appropriate. Pressure P is assigned to be positive whenever a body undergoes hydrostatic compression, per accepted practice.

4.1.1. Constitutive Equations

Because the internal energy density U is a state function, its total derivative describes a Pfaffian form [58] out of which the following constitutive formulæ are readily obtained

$$\text{In 1 Dimension: } \theta = \partial_\eta U(\eta, \ln(L/L_0)) \quad F = \rho_{1D} \partial_{\ln(L/L_0)} U(\eta, \ln(L/L_0)) \quad (4.2a)$$

$$\text{In 2 Dimensions: } \theta = \partial_\eta U(\eta, \ln(A/A_0)) \quad T = \rho_{2D} \partial_{\ln(A/A_0)} U(\eta, \ln(A/A_0)) \quad (4.2b)$$

$$\text{In 3 Dimensions: } \theta = \partial_\eta U(\eta, \ln(V/V_0)) \quad -P = \rho_{3D} \partial_{\ln(V/V_0)} U(\eta, \ln(V/V_0)) \quad (4.2c)$$

where strains are logarithms of dimension-appropriate stretches. As a matter of convenience, we adopt the notation $\partial_\eta U := \partial U / \partial \eta$, etc. Employing the geometric strains of Part 3, viz., $e := \ln(L/L_0)$, $\xi := \ln \sqrt{A/A_0}$ and $\Xi := \ln \sqrt[3]{V/V_0}$ with differential rates of $de = L^{-1} dL$, $d\xi = \frac{1}{2} A^{-1} dA$ and $d\Xi = \frac{1}{3} V^{-1} dV$, these constitutive equations take on the following form

$$\text{In 1 Dimension: } \theta = \partial_\eta U(\eta, e) \quad F = \rho_{1D} \partial_e U(\eta, e) \quad (4.3a)$$

$$\text{In 2 Dimensions: } \theta = \partial_\eta U(\eta, \xi) \quad \pi = \rho_{2D} \partial_\xi U(\eta, \xi) \quad (4.3b)$$

$$\text{In 3 Dimensions: } \theta = \partial_\eta U(\eta, \Xi) \quad \Pi = \rho_{3D} \partial_\Xi U(\eta, \Xi) \quad (4.3c)$$

wherein $\pi := 2T$ and $\Pi := -3P$ are the measures for surface tension and pressure that are used in this work. We find it useful to use this negative measure for pressure because the transpulmonary pressure in lung, under normal physiologic conditions, is typically negative; hence, Π would be positive in its specification of transpulmonary pressure. The above constitutive equations describe Green thermoelastic solids of specified dimension undergoing uniform motions in adiabatic enclosures.

We consider the response variables for temperature and force/surface-tension/pressure to be C^1 functions of state, and therefore, the internal energy U is taken to be a C^2 function of state in Green thermoelastic solids undergoing uniform adiabatic motions (cf. Weinhold [64]

and Gilmore [65]). One can then differentiate Eqn. (4.3), thereby producing the following collection of coupled, partial, differential equations

$$\text{In 1 Dimension: } \begin{Bmatrix} d\theta \\ dF \end{Bmatrix} = \begin{bmatrix} \partial_{\eta\eta} U & \partial_{\eta e} U \\ \rho_{1D} \partial_{e\eta} U & \rho_{1D} \partial_{ee} U \end{bmatrix} \begin{Bmatrix} d\eta \\ de \end{Bmatrix} \quad (4.4a)$$

$$\text{In 2 Dimensions: } \begin{Bmatrix} d\theta \\ d\pi \end{Bmatrix} = \begin{bmatrix} \partial_{\eta\eta} U & \partial_{\eta\xi} U \\ \rho_{2D} \partial_{\xi\eta} U & \rho_{2D} \partial_{\xi\xi} U \end{bmatrix} \begin{Bmatrix} d\eta \\ d\xi \end{Bmatrix} \quad (4.4b)$$

$$\text{In 3 Dimensions: } \begin{Bmatrix} d\theta \\ d\Pi \end{Bmatrix} = \begin{bmatrix} \partial_{\eta\eta} U & \partial_{\eta\Xi} U \\ \rho_{3D} \partial_{\Xi\eta} U & \rho_{3D} \partial_{\Xi\Xi} U \end{bmatrix} \begin{Bmatrix} d\eta \\ d\Xi \end{Bmatrix} \quad (4.4c)$$

where, from calculus, mixed partial derivatives obey $\partial_{e\eta} U = \partial^2 U / \partial e \partial \eta = \partial^2 U / \partial \eta \partial e = \partial_{\eta e} U$, etc., that in the thermodynamics literature are known as Maxwell's relations; they are also known as Silvester's criteria for the integrability of a Pfaffian form.

Exchanging cause and effect between entropy and temperature in Eqn. (4.4) leads to

$$\text{In 1D: } \begin{Bmatrix} d\eta \\ dF \end{Bmatrix} = \begin{bmatrix} 1/\partial_{\eta\eta} U & -\partial_{\eta e} U / \partial_{\eta\eta} U \\ \rho_{1D} \partial_{e\eta} U / \partial_{\eta\eta} U & \rho_{1D} (\partial_{ee} U - \partial_{e\eta} U \cdot \partial_{\eta e} U / \partial_{\eta\eta} U) \end{bmatrix} \begin{Bmatrix} d\theta \\ de \end{Bmatrix} \quad (4.5a)$$

$$\text{In 2D: } \begin{Bmatrix} d\eta \\ d\pi \end{Bmatrix} = \begin{bmatrix} 1/\partial_{\eta\eta} U & -\partial_{\eta\xi} U / \partial_{\eta\eta} U \\ \rho_{2D} \partial_{\xi\eta} U / \partial_{\eta\eta} U & \rho_{2D} (\partial_{\xi\xi} U - \partial_{\xi\eta} U \cdot \partial_{\eta\xi} U / \partial_{\eta\eta} U) \end{bmatrix} \begin{Bmatrix} d\theta \\ d\xi \end{Bmatrix} \quad (4.5b)$$

$$\text{In 3D: } \begin{Bmatrix} d\eta \\ d\Pi \end{Bmatrix} = \begin{bmatrix} 1/\partial_{\eta\eta} U & -\partial_{\eta\Xi} U / \partial_{\eta\eta} U \\ \rho_{3D} \partial_{\Xi\eta} U / \partial_{\eta\eta} U & \rho_{3D} (\partial_{\Xi\Xi} U - \partial_{\Xi\eta} U \cdot \partial_{\eta\Xi} U / \partial_{\eta\eta} U) \end{bmatrix} \begin{Bmatrix} d\theta \\ d\Xi \end{Bmatrix} \quad (4.5c)$$

where we employ the independent variables of a Helmholtz free energy, namely temperature and strain, but we do not adopt his potential, preferring to retain the internal energy potential so as to ensure a proper incorporation of Maxwell's constraint.

Constitutive equations (4.4 & 4.5) take on the form of a hypo-elastic material model [66], which is ideal for numerical implementation whenever one uses solution techniques like those presented in Part 5.

4.1.2. Material Response Functions

Experiments are performed for the purpose of characterizing material behavior. In mechanics, we relate measured material constants to gradients and curvatures of thermodynamic potentials out of which material models are created. Experiments are typically done to quantify the following material constants, selected per a material's physical dimension:

$$C_f := \theta \partial_\theta \eta|_F \quad \alpha_f := L^{-1} \partial_\theta L|_F =: \alpha = \partial_\theta e|_F \quad E_\theta := L \partial_L F|_\theta = \partial_e F|_\theta \quad (4.6a)$$

$$C_t := \theta \partial_\theta \eta|_T \quad \alpha_t := A^{-1} \partial_\theta A|_T = 2\alpha = 2 \partial_\theta \xi|_T \quad M_\theta := A \partial_A T|_\theta = \frac{1}{4} \partial_\xi \pi|_\theta \quad (4.6b)$$

$$C_p := \theta \partial_\theta \eta|_P \quad \alpha_p := V^{-1} \partial_\theta V|_P = 3\alpha = 3 \partial_\theta \Xi|_P \quad K_\theta := -V \partial_V P|_\theta = \frac{1}{9} \partial_\Xi \Pi|_\theta \quad (4.6c)$$

where we employ the commonly used notation $\partial_\theta \eta|_F := (\partial \eta / \partial \theta)|_F$, etc. The various specific heats C_f, C_t, C_p (erg/gr.K) introduced here are, essentially, all equivalent as they are all defined per unit mass, insensitive to dimension. They are evaluated at a fixed thermodynamic force, which does depend on dimension, but this does not impact the value for

specific heat. Hereafter they will be denoted simply as C . The various thermal expansions α_f , α_t , α_p ($1/K$) are, however, all distinct as they are each defined with respect to their physical dimension, viz., $\alpha_f := L^{-1} \partial L / \partial \theta|_F$, $\alpha_t := A^{-1} \partial A / \partial \theta|_T$ and $\alpha_p := V^{-1} \partial V / \partial \theta|_P$. Nevertheless, they relate to one another because $\ln \sqrt{A/A_0} = \ln(L/L_0) \implies \alpha_t = 2\alpha_f$ and $\ln \sqrt[3]{V/V_0} = \ln(L/L_0) \implies \alpha_p = 3\alpha_f$ for uniform motions. Hereafter, only the linear coefficient for thermal expansion, denoted as $\alpha := \alpha_f$, will be used. Parameter E_θ is a modulus of extension (dyne), parameter M_θ is a modulus of dilation (dyne/cm), and parameter K_θ is a modulus of dilatation (dyne/cm²), a.k.a. the bulk modulus, with each modulus being measured at fixed temperature. Shear moduli are discussed later in §4.2 and §4.3. The above material constants are gradients; they constitute tangents to their associated physical response curves. Consequently, they need not be of constant value throughout state space, like a Hookean material would suppose them to be. This is an important characteristic for our application.

In terms of the material constants given in Eqn. (4.6), of which there are three per dimension, the internal energy density has the following three curvatures associated with it. For 1D materials:

$$\partial_{\eta\eta} U = \frac{\rho_{1D} \theta}{\rho_{1D} C - \alpha^2 \theta E_\theta} \quad (4.7a)$$

$$\partial_{ee} U = \frac{CE_\theta}{\rho_{1D} C - \alpha^2 \theta E_\theta} \quad (4.7b)$$

$$\partial_{\eta e} U \equiv \partial_{e\eta} U = \frac{-\alpha \theta E_\theta}{\rho_{1D} C - \alpha^2 \theta E_\theta} \quad (4.7c)$$

For 2D materials:

$$\partial_{\eta\eta} U = \frac{\rho_{2D} \theta}{\rho_{2D} C - 4\alpha^2 \theta M_\theta} \quad (4.7d)$$

$$\partial_{\xi\xi} U = \frac{4CM_\theta}{\rho_{2D} C - 4\alpha^2 \theta M_\theta} \quad (4.7e)$$

$$\partial_{\eta\xi} U \equiv \partial_{\xi\eta} U = \frac{-4\alpha \theta M_\theta}{\rho_{2D} C - 4\alpha^2 \theta M_\theta} \quad (4.7f)$$

For 3D materials (cf. Weinhold [64] and Gilmore [65]):

$$\partial_{\eta\eta} U = \frac{\rho_{3D} \theta}{\rho_{3D} C - 9\alpha^2 \theta K_\theta} \quad (4.7g)$$

$$\partial_{\Xi\Xi} U = \frac{9CK_\theta}{\rho_{3D} C - 9\alpha^2 \theta K_\theta} \quad (4.7h)$$

$$\partial_{\eta\Xi} U \equiv \partial_{\Xi\eta} U = \frac{-9\alpha \theta K_\theta}{\rho_{3D} C - 9\alpha^2 \theta K_\theta} \quad (4.7i)$$

These materials constants are constrained by thermodynamics in that

$$0 < E_\theta < \frac{\rho_{1D} C}{\alpha^2 \theta}, \quad 0 < M_\theta < \frac{\rho_{2D} C}{4\alpha^2 \theta}, \quad 0 < K_\theta < \frac{\rho_{3D} C}{9\alpha^2 \theta} \quad (4.8)$$

which ensure that their respective thermodynamic Jacobians cannot become singular. Singularities can and do occur, e.g., during a phase change in a crystal [53, 65], but such processes are not expected to arise in our application.

4.1.3. Thermoelastic Models Suitable for Modeling Alveoli Subjected to Uniform Motions

We now write down our constitutive formulæ for quantifying uniform responses in thermoelastic solids of 1, 2 and 3 dimensions. They are thermoelastic constitutive equations (4.5) with Helmholtz variables expressed in terms of the material constants defined in Eqn. (4.6) assigned to the internal energy density U according to Eqn. (4.7), with outcomes of:

$$\text{For 1D Materials: } \begin{Bmatrix} d\eta \\ dF \end{Bmatrix} = \begin{bmatrix} C/\theta - \alpha^2 E/\rho & \alpha E/\rho \\ -\alpha E & E \end{bmatrix} \begin{Bmatrix} d\theta \\ de \end{Bmatrix} \quad (4.9a)$$

$$\text{For 2D Materials: } \begin{Bmatrix} d\eta \\ d\pi \end{Bmatrix} = \begin{bmatrix} C/\theta - 4\alpha^2 M/\rho & 4\alpha M/\rho \\ -4\alpha M & 4M \end{bmatrix} \begin{Bmatrix} d\theta \\ d\xi \end{Bmatrix} \quad (4.9b)$$

$$\text{For 3D Materials: } \begin{Bmatrix} d\eta \\ d\Pi \end{Bmatrix} = \begin{bmatrix} C/\theta - 9\alpha^2 K/\rho & 9\alpha K/\rho \\ -9\alpha K & 9K \end{bmatrix} \begin{Bmatrix} d\theta \\ d\Xi \end{Bmatrix} \quad (4.9c)$$

where we simplify our expressions by suppressing the notation specifying that the moduli are evaluated at constant temperature, and by suppressing the dimension for which mass density applies. These are considered to be understood. There are four material constants for each dimension (e.g., for 1D materials they are: ρ , C , α and E) with the latter three constants being defined according to Eqn. (4.6).

The upper-left element in each matrix of Eqn. (4.9) represents a specific heat evaluated at constant strain, divided by temperature—a material property not easily measured. Whereas, the specific heat evaluated at constant pressure, viz., C , is more amenable to experiments, and is the property that one typically finds in published data tables.

Constitutive equations (4.9), derived from the First and Second Laws of Thermodynamics, describe thermoelastic materials undergoing uniform motions through adiabatic processes. They present themselves as hypo-elastic material models [66], which are typically preferred for incorporating constitutive equations into finite element packages.

Equation (4.9) has cause and effect variables that are appropriate for our multiscale application. In this process, a localization procedure pulls the temperature θ and deformation gradient \mathbf{F} taken from the parenchyma scale (Gauss points in a finite element grid of lung) down to that of an alveolar scale (in our modeling, a dodecahedron). Differential strain rates $d\mathcal{U} \cdot \mathcal{U}^{-1}$ are then constructed through appropriate finite difference formulæ, where \mathcal{U} denotes the Laplace stretch [42]. These continuum rates are then mapped into our local thermodynamic rates, with alveolar entropy and stress following from a numerical integration of the above constitutive equations. These constitutive equations apply to the various facets of our dodecahedral model for an alveolar sac through a finite element discretization. Afterwards, an homogenization procedure takes the updated alveolar entropy and nodal tractions, and push them up to the continuum level as parenchymal entropy and stress.

4.2. Green Thermoelastic Membranes Subjected to Non-Uniform Motions

The First and Second Laws of Thermodynamics governing a reversible adiabatic process are described by the formula $dU = \theta d\eta + \frac{1}{\rho} dW$, where dW is the mechanical power expended by stressing a body of mass density ρ . For the case of a 2D planar membrane, a mass density of $\rho \ll \rho_{2D}$ applies, with its change in mechanical work being expressed as [51, 52, 67]

$$dW = \text{tr} \left(\begin{bmatrix} \mathcal{S}_{11} & \mathcal{S}_{12} \\ \mathcal{S}_{21} & \mathcal{S}_{22} \end{bmatrix} \begin{bmatrix} a^{-1} da & (a/b) dg \\ 0 & b^{-1} db \end{bmatrix} \right) = \pi d\xi + \sigma d\varepsilon + \tau d\gamma \quad (4.10a)$$

wherein \mathcal{S}_{ij} are the components of a surface tension evaluated in the co-ordinate frame of a membrane. (In §4.5 they will be converted into components of an Eulerian Kirchhoff stress or a Lagrangian, second, Piola-Kirchhoff stress.)

Equation (4.10a) conjectures that the First and Second Laws of Thermodynamics can be expressed as a differential equation known as a Pfaffian form that, in this case, looks like

$$dU = \theta d\eta + \frac{1}{\rho} (\pi d\xi + \sigma d\varepsilon + \tau d\gamma) \quad (4.10b)$$

where $\{\pi, \sigma, \tau\}$ describes a set of intensive scalar-valued stresses whose thermodynamic conjugates $\{\xi, \varepsilon, \gamma\}$ describe a set of extensive scalar-valued strains. This contrasts with the classic approach where the work done is decomposed into a scalar-valued isotropic part and a tensor-valued deviatoric part. The above thermodynamic strains are defined in §3.3.5.1, while their conjugate stresses, and how they relate to the tensor components of stress, are discussed in §4.5.

Conjugate pair (ξ, π) describes a dilation $2d\xi \ll A^{-1} dA$ caused by a surface tension $\pi \ll 2T$ where $\xi = \ln \sqrt{A/A_0}$ and $\pi = \mathcal{S}_{11} + \mathcal{S}_{22}$. This pair describes the uniform contribution to stress power discussed in §4.1. Pair (ε, σ) describes a pure shear ε or squeeze caused by a normal-stress difference $\sigma = \mathcal{S}_{11} - \mathcal{S}_{22}$. And pair (γ, τ) describes an in-plane shear γ caused by a shear stress τ . Collectively, pairs (ε, σ) and (γ, τ) account for any non-uniform contributions to stress power, i.e., contributions from other than uniform dilation. These pairs are quantified in §4.4.3.

4.2.1. General Constitutive Equations

Because a change in the internal energy dU governing a reversible adiabatic process is described by an exact differential [58], with $U(\eta, \xi, \varepsilon, \gamma)$ in the case of a planar membrane, it follows that a constitutive response for a Green thermoelastic membrane is described by

$$\begin{aligned} \theta &= \partial_\eta U(\eta, \xi, \varepsilon, \gamma) & \pi &= \rho \partial_\xi U(\eta, \xi, \varepsilon, \gamma) \\ \sigma &= \rho \partial_\varepsilon U(\eta, \xi, \varepsilon, \gamma) & \tau &= \rho \partial_\gamma U(\eta, \xi, \varepsilon, \gamma). \end{aligned} \quad (4.11)$$

Considering each intensive variable, viz., θ , π , σ and τ , to be at least a C^1 function of the set of extensive variables $(\eta, \xi, \varepsilon, \gamma)$, thereby implies that the internal energy U is at least a

C^2 function of state, and therefore the constitutive expressions in Eqn. (4.11) can be recast into the following system of differential equations

$$\begin{Bmatrix} d\theta \\ d\pi \\ d\sigma \\ d\tau \end{Bmatrix} = \begin{bmatrix} \partial_{\eta\eta}U & \partial_{\eta\xi}U & \partial_{\eta\varepsilon}U & \partial_{\eta\gamma}U \\ \rho\partial_{\xi\eta}U & \rho\partial_{\xi\xi}U & \rho\partial_{\xi\varepsilon}U & \rho\partial_{\xi\gamma}U \\ \rho\partial_{\varepsilon\eta}U & \rho\partial_{\varepsilon\xi}U & \rho\partial_{\varepsilon\varepsilon}U & \rho\partial_{\varepsilon\gamma}U \\ \rho\partial_{\gamma\eta}U & \rho\partial_{\gamma\xi}U & \rho\partial_{\gamma\varepsilon}U & \rho\partial_{\gamma\gamma}U \end{bmatrix} \begin{Bmatrix} d\eta \\ d\xi \\ d\varepsilon \\ d\gamma \end{Bmatrix} \quad (4.12)$$

whose upper-left 2×2 sub-matrix also appears in Eqn. (4.4b), which governs the uniform contribution of a response. The above 4×4 matrix describes the full non-uniform response permissible by a Green thermoelastic membrane undergoing an adiabatic process.

For our application, it is reasonable to assume that the presence of a non-uniform planar motion will not cause an uniform planar response. Said differently, it is reasonable to assume that pure ε and simple γ shears will not effect a change in either temperature θ or surface tension π . Consequently, $\partial_{\eta\varepsilon}U = \partial_{\eta\gamma}U = \partial_{\xi\varepsilon}U = \partial_{\xi\gamma}U = 0$, and Eqn. (4.12) simplifies to

$$\begin{Bmatrix} d\theta \\ d\pi \\ d\sigma \\ d\tau \end{Bmatrix} = \begin{bmatrix} \partial_{\eta\eta}U & \partial_{\eta\xi}U & 0 & 0 \\ \rho\partial_{\xi\eta}U & \rho\partial_{\xi\xi}U & 0 & 0 \\ 0 & 0 & \rho\partial_{\varepsilon\varepsilon}U & \rho\partial_{\varepsilon\gamma}U \\ 0 & 0 & \rho\partial_{\gamma\varepsilon}U & \rho\partial_{\gamma\gamma}U \end{bmatrix} \begin{Bmatrix} d\eta \\ d\xi \\ d\varepsilon \\ d\gamma \end{Bmatrix}$$

with $\partial_{\varepsilon\eta}U = \partial_{\gamma\eta}U = \partial_{\varepsilon\xi}U = \partial_{\gamma\xi}U = 0$ because of Maxwell's relationships. Furthermore, it is considered that the pure and simple shear responses act independently, too, so that $\partial_{\gamma\varepsilon}U = \partial_{\varepsilon\gamma}U = 0$.⁶ Converting the above internal energy formulation into its Helmholtz equivalent produces two uncoupled matrix equations; they are,

$$\begin{Bmatrix} d\eta \\ d\pi \end{Bmatrix} = \begin{bmatrix} 1/\partial_{\eta\eta}U & -\partial_{\eta\xi}U/\partial_{\eta\eta}U \\ \rho\partial_{\xi\eta}U/\partial_{\eta\eta}U & \rho(\partial_{\xi\xi}U - \partial_{\xi\eta}U \cdot \partial_{\eta\xi}U/\partial_{\eta\eta}U) \end{bmatrix} \begin{Bmatrix} d\theta \\ d\xi \end{Bmatrix} \quad (4.13a)$$

and

$$\begin{Bmatrix} d\sigma \\ d\tau \end{Bmatrix} = \rho \begin{bmatrix} \partial_{\varepsilon\varepsilon}U & 0 \\ 0 & \partial_{\gamma\gamma}U \end{bmatrix} \begin{Bmatrix} d\varepsilon \\ d\gamma \end{Bmatrix} \quad (4.13b)$$

that, collectively, provide a general theoretical structure for a Green thermoelastic membrane appropriate for our application.

Note: The uniform response (Eqn. 4.13a) and the non-uniform response (Eqn. 4.13b) are, by supposition, decoupled in this constitutive construction. There is experimental evidence that the bulk and shear moduli of parenchyma both depend upon transpulmonary pressure [68, 69]. It is conjectured that this is a structural effect of alveolar geometry; it is not a characteristic of the constituents that comprise an alveolus. As such, we do not couple the uniform and non-uniform responses in the constitutive framework of Eqn. (4.13).

⁶There is a second-order coupling that can exist between the modes of squeeze and shear in a 3D solid. It is the Poynting effect [52], but this effect does not arise in a 2D membrane.

4.2.2. Material Response Functions

The material model put forward here for a thermoelastic membrane has six material constants/functions: a mass density ρ , a specific heat C at constant tension, a coefficient for linear thermal expansion α at constant tension, an areal modulus M at constant temperature (2D version of a bulk modulus), a squeeze modulus N , and a shear modulus G at constant squeeze. The specific heat C is defined as

$$C := \theta \partial_\theta \eta|_T = \theta \partial_\theta \eta|_{\frac{1}{2}(\mathcal{S}_{11} + \mathcal{S}_{22})} = \theta \partial_\theta \eta|_\pi \quad (4.14a)$$

where θ is temperature, η is entropy, and $\pi = \mathcal{S}_{11} + \mathcal{S}_{22} = 2T$ is the surface tension acting in a membrane. C is commonly referred to in the literature as the specific heat at constant pressure. The coefficient for linear thermal expansion α is defined as

$$\alpha := L^{-1} \partial_\theta L|_T = \frac{1}{2} A^{-1} \partial_\theta A|_T = \partial_\theta \xi|_\pi \quad (4.14b)$$

where $A = ab$ denotes a relative area with $\xi = \ln \sqrt{A/A_0}$ being the areal strain, a.k.a. dilation, whose associated areal modulus M is defined as

$$M := A \partial_A T|_\theta = A \partial_A \frac{1}{2}(\mathcal{S}_{11} + \mathcal{S}_{22})|_\theta = \frac{1}{4} \partial_\xi \pi|_\theta \quad (4.14c)$$

which is a 2D version of the bulk modulus. The in-plane squeeze modulus N is defined as

$$N := \Gamma \partial_\Gamma N_1 = \Gamma \partial_\Gamma (\mathcal{S}_{11} - \mathcal{S}_{22}) = \frac{1}{2} \partial_\varepsilon \sigma \quad (4.14d)$$

where $\sigma = \mathcal{S}_{11} - \mathcal{S}_{22}$ is the normal-stress difference, often denoted as N_1 in the literature, and where $\Gamma = a/b$ is the stretch of squeeze with $\varepsilon = \ln \sqrt{\Gamma/\Gamma_0}$ being the strain of squeeze. Finally, an in-plane shear modulus G is defined as

$$G := \Gamma \partial_g \mathcal{S}_{21}|_\Gamma = \partial_\gamma \tau|_\Gamma = \partial_\gamma \tau|_\varepsilon \quad (4.14e)$$

where $\tau = \Gamma \mathcal{S}_{21}$ determines the shear stress, with $\gamma = g - g_0$ establishing the shear strain.

4.2.3. Constitutive Equations Governing a Thermoelastic Membrane

It is the Gibbs free-energy potential (viz., $\mathcal{G}(\theta, \pi, \sigma, \tau) = U - \theta\eta - \pi\xi - \sigma\varepsilon - \tau\gamma$, which exchanges cause and effect from that of the internal energy $U(\eta, \xi, \varepsilon, \gamma)$) that is most easily expressed in terms of the above material functions; specifically,

$$\begin{Bmatrix} d\eta \\ d\xi \\ d\varepsilon \\ d\gamma \end{Bmatrix} = - \begin{bmatrix} \partial_{\theta\theta}\mathcal{G} & \partial_{\theta\pi}\mathcal{G} & 0 & 0 \\ \rho \partial_{\pi\theta}\mathcal{G} & \rho \partial_{\pi\pi}\mathcal{G} & 0 & 0 \\ 0 & 0 & \rho \partial_{\sigma\sigma}\mathcal{G} & 0 \\ 0 & 0 & 0 & \rho \partial_{\tau\tau}\mathcal{G} \end{bmatrix} \begin{Bmatrix} d\theta \\ d\pi \\ d\sigma \\ d\tau \end{Bmatrix}$$

where $\partial_{\theta\pi}\mathcal{G} = \partial_{\pi\theta}\mathcal{G}$ from Maxwell's constraint. Incorporating the material constant definitions put forward in Eqn. (4.14) into the above differential equation leads to

$$\begin{Bmatrix} d\eta \\ d\xi \\ d\varepsilon \\ d\gamma \end{Bmatrix} = \begin{bmatrix} C/\theta & \alpha/\rho & 0 & 0 \\ \alpha & 1/4M & 0 & 0 \\ 0 & 0 & 1/2N & 0 \\ 0 & 0 & 0 & 1/G \end{bmatrix} \begin{Bmatrix} d\theta \\ d\pi \\ d\sigma \\ d\tau \end{Bmatrix}$$

because $\partial_{\theta\theta}\mathcal{G} = \partial\eta/\partial\theta$, $\rho\partial_{\pi\theta}\mathcal{G} = \partial\xi/\partial\theta = \rho\partial_{\theta\pi}\mathcal{G}$ and $\rho\partial_{\pi\pi}\mathcal{G} = \partial\xi/\partial\pi = (\partial\pi/\partial\xi)^{-1}$, where gradients $\partial\eta/\partial\theta$, $\partial\xi/\partial\theta$ and $\partial\pi/\partial\xi$, which relate to the material constants/functions defined in Eqn. (4.14). The upper-left 2×2 sub-matrix, which describes the uniform contribution to a response, can be rearranged to read as

$$\begin{Bmatrix} d\eta \\ d\pi \end{Bmatrix} = \begin{bmatrix} C/\theta - 4\alpha^2 M/\rho & 4\alpha M/\rho \\ -4\alpha M & 4M \end{bmatrix} \begin{Bmatrix} d\theta \\ d\xi \end{Bmatrix} \quad (4.15a)$$

while the non-uniform or shear response of Eqn. (4.13b) is described quite simply by

$$\begin{Bmatrix} d\sigma \\ d\tau \end{Bmatrix} = \begin{bmatrix} 2N & 0 \\ 0 & G \end{bmatrix} \begin{Bmatrix} d\varepsilon \\ d\gamma \end{Bmatrix} \quad (4.15b)$$

that, collectively, are used herein to describe a thermoelastic membrane.

4.2.3.1. The Poisson Effect

The areal modulus M is ideally determined from an equibiaxial experiment. Assuming knowledge of its value, then given the following definition for Poisson's ratio

$$\nu := -\frac{db/b}{da/a}$$

it follows that the squeeze modulus N can be determined from an uniaxial experiment where traction is applied along that axis from which elongation a is measured; specifically,

$$N = 2M \frac{1-\nu}{1+\nu} \quad \text{provided that } S_{11} \neq 0 \quad \text{and} \quad S_{21} = S_{22} = 0$$

provided that temperature θ is held constant. Consequently, $\frac{2}{3}M \leq N \leq 2M$ provided that $0 \leq \nu \leq 1/2$, so the squeeze modulus N plays an analogous role to the shear modulus μ found in the classical theory of elasticity.

If one were to consider such a membrane as having uniform thickness h that varies with deformation so as to preserve its volume, then $\nu = 1/2$ and Eqn. (4.15b) would become

$$\begin{Bmatrix} d\sigma \\ d\tau \end{Bmatrix} = \begin{bmatrix} 4M/3 & 0 \\ 0 & G \end{bmatrix} \begin{Bmatrix} d\varepsilon \\ d\gamma \end{Bmatrix} \quad (4.15c)$$

which is the general constitutive structure we adopt for describing alveolar membranes.

Note: The conjugate pair approach presented here allows for a distinct shear modulus G that can take on any positive value. This is important because shear experiments done on soft tissues, which unfortunately are few in number, tend to produce shear moduli that are many orders in magnitude smaller than their bulk moduli, e.g., in parenchyma their ratio is $K/G \approx 10^4$ (150 MPa vs. 10–54 kPa [70]). Classically, such a result has been used to argue that the material can be modeled, to a reasonable approximation, as being ideally incompressible—a 3D notion. Such an assumption is no longer necessary in our formulation.

4.3. Green Thermoelastic 3D Solids Subjected to Non-Uniform Motions

The First and Second Laws of Thermodynamics governing a reversible adiabatic process done on a 3D body result in the formula $dU = \theta d\eta + \frac{1}{\rho} dW$, where dW is the mechanical power expended by stressing a body with mass density ρ , specifically [51, 52, 67]

$$\begin{aligned} dW &= \text{tr} \left(\begin{bmatrix} \mathcal{S}_{11} & \mathcal{S}_{12} & \mathcal{S}_{13} \\ \mathcal{S}_{21} & \mathcal{S}_{22} & \mathcal{S}_{23} \\ \mathcal{S}_{31} & \mathcal{S}_{32} & \mathcal{S}_{33} \end{bmatrix} \begin{bmatrix} a^{-1} da & (a/b) d\gamma & (a/c)(d\beta - \alpha d\gamma) \\ 0 & b^{-1} db & (b/c) d\alpha \\ 0 & 0 & c^{-1} dc \end{bmatrix} \right) \\ &= \Pi d\Xi + \sum_{i=1}^3 (\sigma_i d\varepsilon_i + \tau_i d\gamma_i) \end{aligned} \quad (4.16a)$$

which is subject to constraints $\sigma_3 = -(\sigma_1 + \sigma_2)$ and $d\varepsilon_3 = -(d\varepsilon_1 + d\varepsilon_2)$. Stress components \mathcal{S}_{ij} can be either rotated into the Kirchhoff stress of an Eulerian frame, or they can be pulled back into the second Piola-Kirchhoff stress of a Lagrangian frame, as established in §4.5.

The above expression conjectures that thermodynamics can be described by a Pfaffian equation of the form

$$dU = \theta d\eta + \frac{1}{\rho} \left(\Pi d\Xi + \sum_{i=1}^2 \sigma_i d\varepsilon_i + (\sigma_1 + \sigma_2)(d\varepsilon_1 + d\varepsilon_2) + \sum_{i=1}^3 \tau_i d\gamma_i \right) \quad (4.16b)$$

where stresses $\{\Pi, \sigma_1, \sigma_2, \tau_1, \tau_2, \tau_3\}$ describe a set of independent, scalar-valued, intensive variables, and where strains $\{\Xi, \varepsilon_1, \varepsilon_2, \gamma_1, \gamma_2, \gamma_3\}$ describe a set of independent, scalar-valued, extensive variables. This contrasts with the classic approach where the work done decomposes into a scalar-valued isotropic part and a tensor-valued deviatoric part. A direct consequence of adopting a triangular construction for strain rate is that the pure- and simple-shear contributions of a deviatoric response can be separated into independent scalar contributions; whereas, they remain coupled as a tensor contribution whenever a symmetric construction for strain rate is adopted, which is standard practice today. The above thermodynamic strains are defined in §3.4.2, while their conjugate stresses and how they relate to commonly used stress tensors are discussed later in §4.5.

4.3.1. Constitutive Equations

Because a change in the internal energy dU governing a reversible adiabatic process is described by an exact differential [58], with $U(\eta, \Xi, \varepsilon_1, \varepsilon_2, \gamma_1, \gamma_2, \gamma_3)$ in three space, it follows that a constitutive response for a Green thermoelastic solid is governed by [57]

$$\theta = \partial_\eta U(\eta, \Xi, \varepsilon_1, \varepsilon_2, \gamma_1, \gamma_2, \gamma_3) \quad (4.17a)$$

$$\Pi = \rho \partial_\Xi U(\eta, \Xi, \varepsilon_1, \varepsilon_2, \gamma_1, \gamma_2, \gamma_3) \quad (4.17b)$$

$$\begin{Bmatrix} \sigma_1 \\ \sigma_2 \end{Bmatrix} = \frac{1}{3} \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} \begin{Bmatrix} \rho \partial_{\varepsilon_1} U(\eta, \Xi, \varepsilon_1, \varepsilon_2, \gamma_1, \gamma_2, \gamma_3) \\ \rho \partial_{\varepsilon_2} U(\eta, \Xi, \varepsilon_1, \varepsilon_2, \gamma_1, \gamma_2, \gamma_3) \end{Bmatrix} \quad (4.17c)$$

$$\tau_1 = \rho \partial_{\gamma_1} U(\eta, \Xi, \varepsilon_1, \varepsilon_2, \gamma_1, \gamma_2, \gamma_3) \quad (4.17d)$$

$$\tau_2 = \rho \partial_{\gamma_2} U(\eta, \Xi, \varepsilon_1, \varepsilon_2, \gamma_1, \gamma_2, \gamma_3) \quad (4.17e)$$

$$\tau_3 = \rho \partial_{\gamma_3} U(\eta, \Xi, \varepsilon_1, \varepsilon_2, \gamma_1, \gamma_2, \gamma_3) \quad (4.17f)$$

where the coupled expression for the two squeeze stresses arises from the contribution

$$\partial_{\varepsilon_1} U d\varepsilon_1 + \partial_{\varepsilon_2} U d\varepsilon_2 = \sigma_1 d\varepsilon_1 + \sigma_2 d\varepsilon_2 + (\sigma_1 + \sigma_2)(d\varepsilon_1 + d\varepsilon_2)$$

that incorporates constraints $\sigma_3 = -(\sigma_1 + \sigma_2)$ and $d\varepsilon_3 = -(d\varepsilon_1 + d\varepsilon_2)$ into the work done, viz., $\sigma_3 d\varepsilon_3$ does work, and as such, conjugate pair $(\sigma_3, \varepsilon_3)$ has an influence on constitutive response.

Considering each independent intensive variable, viz., θ , Π , σ_1 , σ_2 , τ_1 , τ_2 and τ_3 , to be at least a C^1 function of the set of independent extensive variables $(\eta, \Xi, \varepsilon_1, \varepsilon_2, \gamma_1, \gamma_2, \gamma_3)$, then the internal energy U must be at least a C^2 function of state and the constitutive expressions in Eqn. (4.17) can be recast into the following system of differential equations

$$\begin{Bmatrix} d\theta \\ d\Pi \\ d\sigma_1 \\ d\sigma_2 \\ d\tau_1 \\ d\tau_2 \\ d\tau_3 \end{Bmatrix} = \begin{bmatrix} \partial_{\eta\eta} U & \partial_{\eta\Xi} U & \partial_{\eta\varepsilon_1} U & \partial_{\eta\varepsilon_2} U & \partial_{\eta\gamma_1} U & \partial_{\eta\gamma_2} U & \partial_{\eta\gamma_3} U \\ \rho \partial_{\Xi\eta} U & \rho \partial_{\Xi\Xi} U & \rho \partial_{\Xi\varepsilon_1} U & \rho \partial_{\Xi\varepsilon_2} U & \rho \partial_{\Xi\gamma_1} U & \rho \partial_{\Xi\gamma_2} U & \rho \partial_{\Xi\gamma_3} U \\ \rho M_{1\eta} & \rho M_{1\Xi} & \rho M_{1\varepsilon_1} & \rho M_{1\varepsilon_2} & \rho M_{1\gamma_1} & \rho M_{1\gamma_2} & \rho M_{1\gamma_3} \\ \rho M_{2\eta} & \rho M_{2\Xi} & \rho M_{2\varepsilon_1} & \rho M_{2\varepsilon_2} & \rho M_{2\gamma_1} & \rho M_{2\gamma_2} & \rho M_{2\gamma_3} \\ \rho \partial_{\gamma_1\eta} U & \rho \partial_{\gamma_1\Xi} U & \rho \partial_{\gamma_1\varepsilon_1} U & \rho \partial_{\gamma_1\varepsilon_2} U & \rho \partial_{\gamma_1\gamma_1} U & \rho \partial_{\gamma_1\gamma_2} U & \rho \partial_{\gamma_1\gamma_3} U \\ \rho \partial_{\gamma_2\eta} U & \rho \partial_{\gamma_2\Xi} U & \rho \partial_{\gamma_2\varepsilon_1} U & \rho \partial_{\gamma_2\varepsilon_2} U & \rho \partial_{\gamma_2\gamma_1} U & \rho \partial_{\gamma_2\gamma_2} U & \rho \partial_{\gamma_2\gamma_3} U \\ \rho \partial_{\gamma_3\eta} U & \rho \partial_{\gamma_3\Xi} U & \rho \partial_{\gamma_3\varepsilon_1} U & \rho \partial_{\gamma_3\varepsilon_2} U & \rho \partial_{\gamma_3\gamma_1} U & \rho \partial_{\gamma_3\gamma_2} U & \rho \partial_{\gamma_3\gamma_3} U \end{bmatrix} \begin{Bmatrix} d\eta \\ d\Xi \\ d\varepsilon_1 \\ d\varepsilon_2 \\ d\gamma_1 \\ d\gamma_2 \\ d\gamma_3 \end{Bmatrix} \quad (4.18)$$

whose upper-left 2×2 sub-matrix also appears in Eqn. (4.4c), which governs the uniform contribution of a response. The squeeze response of Eqn. (4.17c) associates with tangent moduli that are defined accordingly

$$M_{1\eta} = \frac{1}{3}(2\partial_{\varepsilon_1\eta} U - \partial_{\varepsilon_2\eta} U) \quad (4.19a)$$

$$M_{1\Xi} = \frac{1}{3}(2\partial_{\varepsilon_1\Xi} U - \partial_{\varepsilon_2\Xi} U) \quad (4.19b)$$

$$M_{1\varepsilon_1} = \frac{1}{3}(2\partial_{\varepsilon_1\varepsilon_1} U - \partial_{\varepsilon_2\varepsilon_1} U) \quad (4.19c)$$

$$M_{1\varepsilon_2} = \frac{1}{3}(2\partial_{\varepsilon_1\varepsilon_2} U - \partial_{\varepsilon_2\varepsilon_2} U) \quad (4.19d)$$

$$M_{1\gamma_1} = \frac{1}{3}(2\partial_{\varepsilon_1\gamma_1} U - \partial_{\varepsilon_2\gamma_1} U) \quad (4.19e)$$

$$M_{1\gamma_2} = \frac{1}{3}(2\partial_{\varepsilon_1\gamma_2} U - \partial_{\varepsilon_2\gamma_2} U) \quad (4.19f)$$

$$M_{1\gamma_3} = \frac{1}{3}(2\partial_{\varepsilon_1\gamma_3} U - \partial_{\varepsilon_2\gamma_3} U) \quad (4.19g)$$

so that, collectively, Eqns. (4.18 & 4.19) describe the full non-uniform response permissible by a Green thermoelastic solid expressed as a hypo-elastic material undergoing an adiabatic process.

As in the case of membranes, it is reasonable to assume that the presence of a non-uniform motion will not cause an uniform response. For our application, it is also reasonable to assume that there is no coupling between the modes of squeeze and shear.⁷ Furthermore, it is assumed that there is no coupling betwixt the two independent squeeze modes, nor

⁷The Poynting effect is a second-order effect that couples squeeze and shear [52]. It is assumed that such a coupling does not play a contributing role in the current application, and can therefore be neglected.

between the three independent shear modes. Consequently, all mixed partial derivatives that associate with a non-uniform response are taken to be zero, and therefore Eqns. (4.18 & 4.19) simplify to

$$\begin{Bmatrix} d\theta \\ d\Pi \\ d\sigma_1 \\ d\sigma_2 \\ d\tau_1 \\ d\tau_2 \\ d\tau_3 \end{Bmatrix} = \begin{bmatrix} \partial_{\eta\eta}U & \partial_{\eta\Xi}U & 0 & 0 & 0 & 0 & 0 \\ \rho\partial_{\Xi\eta}U & \rho\partial_{\Xi\Xi}U & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \rho\frac{2}{3}\partial_{\varepsilon_1\varepsilon_1}U & -\rho\frac{1}{3}\partial_{\varepsilon_2\varepsilon_2}U & 0 & 0 & 0 \\ 0 & 0 & -\rho\frac{1}{3}\partial_{\varepsilon_1\varepsilon_1}U & \rho\frac{2}{3}\partial_{\varepsilon_2\varepsilon_2}U & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \rho\partial_{\gamma_1\gamma_1}U & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \rho\partial_{\gamma_2\gamma_2}U & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \rho\partial_{\gamma_3\gamma_3}U \end{bmatrix} \begin{Bmatrix} d\eta \\ d\Xi \\ d\varepsilon_1 \\ d\varepsilon_2 \\ d\gamma_1 \\ d\gamma_2 \\ d\gamma_3 \end{Bmatrix}$$

where what may appear as being a coupling between $d\sigma_1$ and $d\sigma_2$ is actually a consequence arising from the constraint equations $d\sigma_3 = -(d\sigma_1 + d\sigma_2)$ and $d\varepsilon_3 = -(d\varepsilon_1 + d\varepsilon_2)$.

The above system of equations can be rewritten as three independent systems of differential equations; specifically, the first differential matrix equation is

$$\begin{Bmatrix} d\theta \\ d\Pi \end{Bmatrix} = \begin{bmatrix} \partial_{\eta\eta}U & \partial_{\eta\Xi}U \\ \rho\partial_{\Xi\eta}U & \rho\partial_{\Xi\Xi}U \end{bmatrix} \begin{Bmatrix} d\eta \\ d\Xi \end{Bmatrix}$$

that we rewrite in terms of Helmholtz state variables, thereby producing the matrix equation we use to describe an isotropic response

$$\begin{Bmatrix} d\eta \\ d\Pi \end{Bmatrix} = \begin{bmatrix} 1/\partial_{\eta\eta}U & -\partial_{\eta\Xi}U/\partial_{\eta\eta}U \\ \rho(\partial_{\Xi\eta}U/\partial_{\eta\eta}U) & \rho(\partial_{\Xi\Xi}U - \partial_{\Xi\eta}U \cdot \partial_{\eta\Xi}U/\partial_{\eta\eta}U) \end{bmatrix} \begin{Bmatrix} d\theta \\ d\Xi \end{Bmatrix} \quad (4.20a)$$

plus a matrix equation that governs the squeeze response

$$\begin{Bmatrix} d\sigma_1 \\ d\sigma_2 \end{Bmatrix} = \frac{\rho}{3} \begin{bmatrix} 2\partial_{\varepsilon_1\varepsilon_1}U & -\partial_{\varepsilon_2\varepsilon_2}U \\ -\partial_{\varepsilon_1\varepsilon_1}U & 2\partial_{\varepsilon_2\varepsilon_2}U \end{bmatrix} \begin{Bmatrix} d\varepsilon_1 \\ d\varepsilon_2 \end{Bmatrix} \quad (4.20b)$$

and a matrix equation that governs the shear response

$$\begin{Bmatrix} d\tau_1 \\ d\tau_2 \\ d\tau_3 \end{Bmatrix} = \rho \begin{bmatrix} \partial_{\gamma_1\gamma_1}U & 0 & 0 \\ 0 & \partial_{\gamma_2\gamma_2}U & 0 \\ 0 & 0 & \partial_{\gamma_3\gamma_3}U \end{bmatrix} \begin{Bmatrix} d\gamma_1 \\ d\gamma_2 \\ d\gamma_3 \end{Bmatrix} \quad (4.20c)$$

that we now seek to describe in terms of specified material functions.

4.3.2. Material Response Functions

The material model put forward here is for a general thermoelastic solid that has, at most, nine material constants/functions: a mass density ρ , a specific heat C and a coefficient for linear thermal expansion α , both evaluated at constant pressure, a bulk modulus K evaluated at constant temperature, two squeeze moduli N_1 and N_2 , and three shear moduli G_1 , G_2 and G_3 evaluated at constant squeeze. The specific heat C is defined as

$$C := \theta \partial_\theta \eta|_P = \theta \partial_\theta \eta|_{-\frac{1}{3}(S_{11} + S_{22} + S_{33})} = \theta \partial_\theta \eta|_\Pi \quad (4.21a)$$

where θ is temperature, η is entropy, and $\Pi = \mathcal{S}_{11} + \mathcal{S}_{22} + \mathcal{S}_{33} = -3P$ is negative pressure. (Transpulmonary pressure is negative—mean stress is positive—under normal physiologic conditions.) The coefficient for thermal expansion α is defined as

$$\alpha := L^{-1} \partial_\theta L|_P = \frac{1}{3} V^{-1} \partial_\theta V|_P = \partial_\theta \Xi|_\Pi \quad (4.21b)$$

where $V = abc$ denotes a relative volume with $\Xi = \ln \sqrt[3]{V/V_0}$ being volumetric strain, a.k.a. dilatation, whose associated bulk modulus K is defined as

$$K := -V \partial_V P|_\theta = V \partial_V \frac{1}{3}(\mathcal{S}_{11} + \mathcal{S}_{22} + \mathcal{S}_{33})|_\theta = \frac{1}{9} \partial_\Xi \Pi|_\theta \quad (4.21c)$$

that together describe the uniform response. The non-uniform response is described in terms of two in-plane squeeze moduli N_1 and N_2 that are defined as

$$N_1 := \Gamma_1 \partial_{\Gamma_1} (\mathcal{S}_{11} - \mathcal{S}_{22})|_{\Gamma_2} = \frac{1}{3} \partial_{\varepsilon_1} \sigma_1|_{\Gamma_2} \quad (4.21d)$$

$$N_2 := \Gamma_2 \partial_{\Gamma_2} (\mathcal{S}_{22} - \mathcal{S}_{33})|_{\Gamma_1} = \frac{1}{3} \partial_{\varepsilon_2} \sigma_2|_{\Gamma_1} \quad (4.21e)$$

where $\sigma_1 = \mathcal{S}_{11} - \mathcal{S}_{22}$ and $\sigma_2 = \mathcal{S}_{22} - \mathcal{S}_{33}$ are the first and second normal-stress differences, with $\Gamma_1 = a/b$ and $\Gamma_2 = b/c$ being their respective stretches of squeeze with $\varepsilon_1 = \ln \sqrt[3]{\Gamma_1/\Gamma_{10}}$ and $\varepsilon_2 = \ln \sqrt[3]{\Gamma_2/\Gamma_{20}}$ being their strains of squeeze. Finally, there are three in-plane shear moduli G_{ε_1} , G_{ε_2} and G_{ε_3} that are defined as

$$G_1 := \Gamma_2 \partial_{\gamma_1} \mathcal{S}_{32}|_{\Gamma_2} \quad (4.21f)$$

$$G_2 := \Gamma_1 \Gamma_2 \partial_{\gamma_2} \mathcal{S}_{31}|_{\Gamma_1 \Gamma_2} \quad (4.21g)$$

$$G_3 := \Gamma_1 \partial_{\gamma_3} \mathcal{S}_{21}|_{\Gamma_1, \gamma_1, \tau_2} \quad (4.21h)$$

where $\tau_1 = \Gamma_2 \mathcal{S}_{32}$, $\tau_2 = \Gamma_1 \Gamma_2 \mathcal{S}_{31}$ and $\tau_3 = \Gamma_1 \mathcal{S}_{21} - \alpha \tau_2$ quantify the three shear stresses, with $\gamma_1 = \alpha - \alpha_0$, $\gamma_2 = \beta - \beta_0$ and $\gamma_3 = \gamma - \gamma_0$ being their respective shear strains.

A material is said to be ‘isotropic’ in our constitutive framework, like the materials considered in our application, if its squeeze moduli can be described via a single material function, i.e., $N_1 = N(\sigma_1, \varepsilon_1)$ and $N_2 = N(\sigma_2, \varepsilon_2)$, and if its shear moduli can be described via a single material function, viz., $G_1 = G(\tau_1, \gamma_1)$, $G_2 = G(\tau_2, \gamma_2)$ and $G_3 = G(\tau_3, \gamma_3)$. In other words, the two squeeze response curves may have different tangents at any given moment, but these tangents are evaluated from the same material function for squeeze. A like statement applies to shear. An isotropic thermoelastic solid therefore has six material constants/functions: ρ , C , α , K , N and G .

4.3.3. Constitutive Equations Governing a Thermoelastic Solid

In terms of the material constants put forward in Eqn. (4.21), the uniform response of the thermoelastic solid given in Eqn. (4.20a) takes on the form of

$$\begin{Bmatrix} d\eta \\ d\Pi \end{Bmatrix} = \begin{bmatrix} C/\theta - 3\alpha^2 K/\rho & 3\alpha K/\rho \\ -3\alpha K & 9K \end{bmatrix} \begin{Bmatrix} d\theta \\ d\Xi \end{Bmatrix} \quad \text{where} \quad K = K(\theta, \Pi, \Xi) \quad (4.22a)$$

while the non-uniform squeeze response is described by

$$\begin{Bmatrix} d\sigma_1 \\ d\sigma_2 \end{Bmatrix} = \frac{3}{2} \begin{bmatrix} 2N_1 & -N_2 \\ -N_1 & 2N_2 \end{bmatrix} \begin{Bmatrix} d\varepsilon_1 \\ d\varepsilon_2 \end{Bmatrix} \quad \text{where} \quad \begin{aligned} N_1 &= N(\sigma_1, \varepsilon_1) \\ N_2 &= N(\sigma_2, \varepsilon_2) \end{aligned} \quad (4.22b)$$

and the non-uniform shear response is described by

$$\begin{Bmatrix} d\tau_1 \\ d\tau_2 \\ d\tau_3 \end{Bmatrix} = \begin{bmatrix} G_1 & 0 & 0 \\ 0 & G_2 & 0 \\ 0 & 0 & G_3 \end{bmatrix} \begin{Bmatrix} d\gamma_1 \\ d\gamma_2 \\ d\gamma_3 \end{Bmatrix} \quad \text{where} \quad \begin{aligned} G_1 &= G(\tau_1, \gamma_1) \\ G_2 &= G(\tau_2, \gamma_2) \\ G_3 &= G(\tau_3, \gamma_3) \end{aligned} \quad (4.22c)$$

which is the general form for a thermoelastic solid that we shall use going forward.

4.3.3.1. The Poisson Effect

Assuming that the bulk modulus K is known, then the squeeze modulus N for an isotropic material can be determined from a single uniaxial experiment by measuring its Poisson response via

$$\nu := -\frac{db/b}{da/a} = -\frac{dc/c}{da/a}$$

from which it follows that

$$N = 3K \frac{1 - 2\nu}{1 + \nu} \quad \text{provided that } S_{11} \neq 0 \quad \text{and} \quad S_{22} = S_{33} = 0$$

where temperature θ has been held constant. Consequently, $N = 2\mu$ where μ is the shear modulus from the classical theory of elasticity. On the other hand, our shear modulus G is distinct from its classical interpretation μ .

4.4. Modeling an Alveolus

To facilitate the numeric implementation of our models, and to facilitate interpretations of their results by engineers and scientists whom will use our framework, this section converts all fields defined in 1D and 2D into their 3D analogs; specifically, forces and surface tensions are converted into stresses, all moduli will now have units of stress, all coefficients for thermal expansion will now associate with linear expansions, and all mass densities will now relate mass to volume.

Only one-third of the cross-sectional area of an alveolar chord, and only one-half of the wall thickness of an alveolar septum associate with any given dodecahedron [30]. Specifically, a third of the total force carried by a septal fiber belongs with the given alveolus, with the remaining two-thirds of the transmitted force belonging to its two adjoining alveoli. Likewise, only half of the surface traction carried along a septal membrane belongs with the given alveolus, with the other half of its surface traction belonging to its adjacent alveolus. Like statements apply for their entropies.

About 75% of the acting transpulmonary pressure (the difference between pleural and alveolar pressures) is carried by the alveolar structure, with the remaining 25% being carried by the pleural membrane encasing the lung [71].

4.4.1. Constraints/Assumptions for Alveoli Subjected to Shock Waves

Because the primary purpose for the alveolar model being constructed here is to better understand alveolar behavior as a shock wave passes over it, there are certain assumptions that we impose upon our model that under normal or different physiologic conditions might otherwise not apply.

First: An alveolus is considered to be an adiabatic pressure vessel in which air and heat cannot move into or out of as a shock wave passes over it, simply because the wave speed is too fast. There is insufficient time for these transport phenomena to occur.

Second: The tissues that comprise lung are viscoelastic [21, 72]. However, whenever a lung is subjected to a shock wave there is insufficient time for the viscous characteristics in a viscoelastic response to manifest themselves. The overall response remains glassy elastic.

Third: Temperature remains constant across a shock wave-front traveling through a compressible gas [73]. It is therefore assumed that alveolar temperature remains at body temperature whenever a lung is subjected to a shock wave. All changes in alveolar entropy are therefore caused by changes in alveolar strain.

Fourth: The air/membrane interface of an alveolus is lined with a surfactant, which is a thin bi-lipid film that plays a substantial role during normal lung function. This film reduces alveolar surface tension to help advert total lung collapse at maximum exhale [74]. Even so, some alveoli still collapse, getting re-recruited during a later breath. Models have been proposed for both surfactant [75] and alveolar recruitment [76], but these effects are not included here as they are not thought to play a significant role in lung mechanics when subjected to a shock wave.

Fifth: Matsuda *et al.* [77] found the diameters of collagen and elastin fibers that circumscribe an alveolar mouth to be about 5-7 times larger than those of their septal chords. The alveolar mouth, with its thicker fibers and open face that attach an alveolus to an alveolar duct, is modeled here as a phantom face, viz., with fibers sized like any of the other eleven pentagonal elements comprising a dodecahedron, and a twelfth face placed where the alveolar mouth resides [14]. Kimmel & Budiansky supported this conjecture via a private communication they had with Prof. T. A. Wilson. They wrote [32]:

“Professor T. A. Wilson notes that the present model does not take explicit account of either alveolar openings or their fibrous boundaries. Wilson suggests that the elastic resistance of the ring boundaries tends to make up for the missing surface tension in the holes, so that neglect of both effects may be self-compensating.”

This conjecture of Kimmel & Budiansky, along with the experimental findings of Matsuda *et al.*, provides a pathway by which we can scale the surface traction carried by a single alveolar membrane with that of the chords the envelope it. In other words, this provides an avenue for parameterizing the membrane model in an otherwise void of relevant experimental data needed to estimate its parameters.

Sixth: Membranes have elastic moduli plus a bending stiffness excited by curvature. This bending energy is proportional to $(w/r)^2$, with w being membrane thickness (width) and r being its radius of curvature. Consequently, bending stresses can be neglected when compared with their in-plane stresses whenever $w \ll r$, which is the supposition here. This

transpulmonary pressure		4 cm H ₂ O		
Age		15–35	36–45	> 65
collagen: \sqrt{D} , (μm) ^{1/2}		0.952 ± 0.242	0.958 ± 0.255	1.045 ± 0.270
elastin: \sqrt{D} , (μm) ^{1/2}		0.957 ± 0.239	0.970 ± 0.213	1.093 ± 0.274
transpulmonary pressure		14 cm H ₂ O		
Age		15–35	36–45	> 65
collagen: \sqrt{D} , (μm) ^{1/2}		0.955 ± 0.246	0.994 ± 0.237	1.054 ± 0.279
elastin: \sqrt{D} , (μm) ^{1/2}		0.956 ± 0.237	0.988 ± 0.263	1.079 ± 0.281

Table 4.1: Mean and standard deviations in variance for the square root of septal chord diameters \sqrt{D} reported by Sabin *et al.* [41]. These septal chords are comprised of collagen and elastin fibers that act independent of one another, and therefore, they are considered to be loaded in parallel with one another.

is in concert with our assumption that the septal chords are modeled as rods, not beams, because of their slenderness ratio. Furthermore, these septa tend to be flat because there are roughly equal pressures acting on both sides of these membranes, eliminating the driving force behind bending [21] and, we surmise, helping to suppress wrinkling, too.

4.4.2. Modeling Septal Chords Subjected to Shock Waves

Alveoli are biologic structures constructed of septal chords that circumscribe alveolar membranes that envelope an alveolar sac whereat gas exchange occurs. These chords are comprised of individual collagen and elastin fibers loaded in parallel [41, 77]. The extent of elastic energy stored within a chord will depend upon the diameters D^c and D^e and length L of these individual fibers.⁸ Let superscript ‘ c ’ denote collagen, and superscript ‘ e ’ denote elastin. Sabin *et al.* [41] determined that the square root of their diameters \sqrt{D} distribute normally, with a mean $\bar{D}^{1/2}$ and standard deviation $\sigma_{\sqrt{D}}$ that also depend upon age and transpulmonary pressure, as presented in Table 4.1 and illustrated in Fig. 4.1.

The collagen and elastin fibers that make up a septal chord have the same length L , they experience the same strain e , and they exist at the same temperature θ ; therefore, we employ Eqn. (4.9a) as the governing constitutive equation to describe their mechanical behaviors; specifically, for the collagen fiber in an alveolar chord

$$\begin{Bmatrix} d\eta^c \\ ds^c \end{Bmatrix} = \begin{bmatrix} C^c/\theta - (\alpha^c)^2 E^c / \rho^c & \alpha^c E^c / \rho^c \\ -\alpha^c E^c & E^c \end{bmatrix} \begin{Bmatrix} d\theta \\ de \end{Bmatrix} \quad (4.23a)$$

and for the elastin fiber in an alveolar chord

$$\begin{Bmatrix} d\eta^e \\ ds^e \end{Bmatrix} = \begin{bmatrix} C^e/\theta - (\alpha^e)^2 E^e / \rho^e & \alpha^e E^e / \rho^e \\ -\alpha^e E^e & E^e \end{bmatrix} \begin{Bmatrix} d\theta \\ de \end{Bmatrix} \quad (4.23b)$$

⁸Sabin *et al.* [41] considered that the stored energy of chords also depends upon their curvature, which they measured and quantified, i.e., they considered these chords to be beams. However, with a slenderness ratio of $\bar{L}/\bar{D} = 102 \pm 12$, which we obtained from analyzing their data, it is reasonable to model them as rods, not beams. Consequently, the dodecahedral truss used as an alveolar model is considered to be a pinned truss, not a rigid truss, thereby greatly simplifying the boundary value problem.

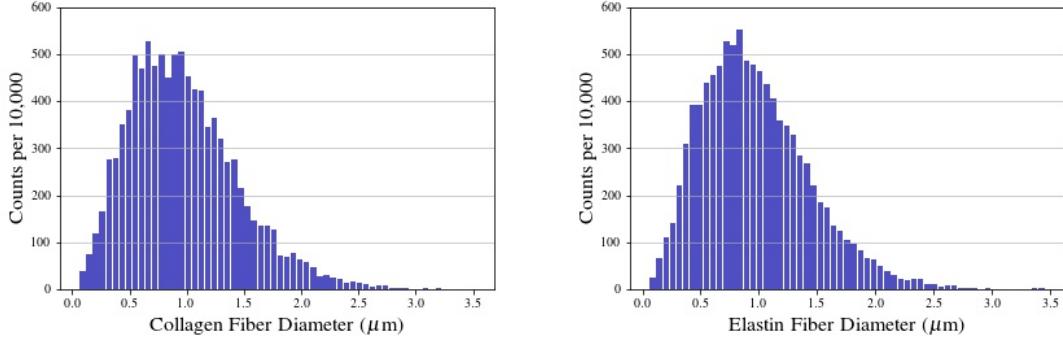


Figure 4.1: Typical histograms for collagen and elastin chord diameters pertaining to the statistics reported in Table 4.1. Their tails weigh heavy at the larger diameters, because their distributions are normal in the square root of their diameters. These histograms are identical, for all practical purposes.

where η^c and η^e are the entropy densities (erg/gr.K) for collagen and elastin; $s^c := \lambda F^c / A_0^c$ and $s^e := \lambda F^e / A_0^e$ are the chordal stresses (barye = dyne/cm²) carried by the collagen and elastin fibers, wherein $\lambda = L/L_0$ is the fiber stretch, A_0^c and A_0^e are their traction-free cross-sectional areas (cm²), and F^c and F^e are the forces (dyne) they transmit. Parameters C^c and C^e are their specific heats at constant pressure (erg/gr.K), α^c and α^e are their linear coefficients of thermal expansion (1/K), E^c and E^e are their elastic moduli (dyne/cm² = erg/cm³), and ρ^c and ρ^e are their mass densities (gr/cm³). These differential equations are subject to initial conditions considered to be $s_0^c = s^c|_{L=L_0} = 0$, $s_0^e = s^e|_{L=L_0} = 0$, $\eta^c = \eta_0^c$ and $\eta^e = \eta_0^e$, where η_0^c and η_0^e are their respective entropy densities at rest.

The actual force and entropy of an individual septal chord in our alveolar model is taken to be one third of a fiber's calculated values, as determined by Eqn. (4.23), because each alveolar chord is typically shared between three adjoining alveoli; consequently,

$$F^f = (A_0^c s^c + A_0^e s^e)/3\lambda \quad \text{and} \quad S^f = (\rho^c V_0^c \eta^c + \rho^e V_0^e \eta^e)/3 \quad (4.24)$$

where F^f (dyne) is a third of the fiber's force carried by a septal chord, and S^f (erg/K) is a third of the fiber's entropy.

Collagen is a fiber comprised of numerous, long, slender, wavy filaments whose waviness, known as crimp, straightens under sufficient deformation [78, 79]. Elastin is a linked fiber network, much like an elastomer, whose filaments between crosslinks rotate to align with an axis of loading under sufficient deformation [80, 81]. Consequently, collagen and elastin both recruit constituent filaments with increasing deformation into an overall, load-bearing, fiber response. The internal energies of collagen and elastin may therefore be thought of as being comprised of a configurational energy and a strain energy. As such, both collagen and elastin are modeled as Freed-Rajagopal biologic fibers, which are described in terms of two such internal energies. Their model is derived from the theory of implicit elasticity in Appendix A. According to their model, tangent compliances for collagen and elastin are

Collagen		
Parameter	Value	Reference
ρ^c [gr/cm ³]	1.34	Fels [82]
η_0^c [erg/gr.K]	3.7×10^7	
C^c [erg/gr.K]	1.7×10^7	Kanagy [83]
α^c [1/C]	1.8×10^{-4}	Weir [84]
e_t^c	0.09	estimated from TLC $\approx 30\%$
E_1^c [barye]	5.0×10^5	authors experience
E_2^c [barye]	3.0×10^7	authors experience
Elastin		
Parameter	Value	Reference
ρ^e [gr/cm ³]	1.31	Lillie & Gosline [85]
η_0^e [erg/gr.K]	3.4×10^7	Shadwick & Gosline [86]
C^e [erg/gr.K]	4.2×10^7	Kakivaya & Hoeve [87]
α^e [1/C]	3.2×10^{-4}	Lillie & Gosline [85]
e_t^e	0.4	Shadwick & Gosline [86]
E_1^e [barye]	2.3×10^6	Urry [81, Fig. 18]
E_2^e [barye]	1.0×10^7	Lillie & Gosline [88, Fig. 5]

Table 4.2: Physical properties for hydrated collagen and elastin fibers. Collagen denatures at around 60°C [89], i.e., above this temperature collagen will shrink rapidly—an effect not modeled here.

described by

$$\frac{1}{E^c(\theta, s^c, e)} = \frac{e_t^c - e_1^c}{E_1^c e_t^c + 2s^c} + \frac{1}{E_2^c} \quad e_1^c = e - \alpha^c(\theta - \theta_0) - \frac{s^c}{E_2^c} \quad (4.25a)$$

$$\frac{1}{E^e(\theta, s^e, e)} = \frac{e_t^e - e_1^e}{E_1^e e_t^e + 2s^e} + \frac{1}{E_2^e} \quad e_1^e = e - \alpha^e(\theta - \theta_0) - \frac{s^e}{E_2^e} \quad (4.25b)$$

where θ_0 is body temperature, i.e., 310 K. Material constants E_1^c and E_2^c are the two asymptotic moduli for collagen that bound its response, i.e., $E_1^c \leq E^c \leq E_2^c$, while E_1^e and E_2^e are the two asymptotic moduli for elastin that bound its response, viz., $E_1^e \leq E^e \leq E_2^e$, both having units of stress (barye = dyne/cm²), with e_t^c and e_t^e being their respective transition strains, cf. Appendix A.

The material properties needed to model septal chords are listed in Tables 4.1 & 4.2. From Eqn. (4.8), these moduli are bound from above by $E_{\max}^c = 4.9 \times 10^9$ barye (dyne/cm²) and $E_{\max}^e = 1.7 \times 10^9$ barye. We therefore observe that E_2^c and E_2^e are about 100 times smaller than E_{\max}^c and E_{\max}^e . We recall that temperature $\theta = \theta_0$ in our application, where θ_0 is body temperature, so strains e_1^c and e_1^e defined in the second column above simplify somewhat.

4.4.3. Modeling Alveolar Septa Subjected to Shock Waves

The thermoelastic response of a planar membrane used to model alveolar septa, as described in Eqn. (4.15), is governed by the following pair of differential equations. The first

set of ODEs establishes the uniform response in Eqn. (4.15a) for a membrane described by

$$\begin{Bmatrix} d\eta \\ ds^\pi \end{Bmatrix} = \begin{bmatrix} C/\theta - 4\alpha^2 M/\rho & 4\alpha M/\rho \\ -4\alpha M & 4M \end{bmatrix} \begin{Bmatrix} d\theta \\ d\xi \end{Bmatrix}$$

while the second set of ODEs establishes the non-uniform response in Eqn. (4.15c) for a membrane described by

$$\begin{Bmatrix} ds^\sigma \\ ds^\tau \end{Bmatrix} = \begin{bmatrix} 4M/3 & 0 \\ 0 & G \end{bmatrix} \begin{Bmatrix} d\varepsilon \\ d\gamma \end{Bmatrix}$$

where $s^\pi := \pi/h$, $s^\sigma := \sigma/h$ and $s^\tau := \tau/h$ have units of stress (dyne/cm^2) with h denoting the height or thickness of a septal membrane that, assuming the volume of a septal membrane remains constant, it is described by $h = h_0 \exp(-2\xi)$ where h_0 is its traction-free thickness.

From a mechanics perspective, we know a great deal more about alveolar chords than we know about alveolar septa. More judgment will therefore be required in our construction and parameterization of a material model for alveolar membranes.

A typical alveolar septum is $4\text{-}5 \mu\text{m}$ in width [62]. They are comprised of an outside layer of epithelial cells that encase capillaries made of endothelial cells along with a basement membrane that is composed of unorganized collagen and elastin filaments, plus proteoglycans and other extracellular proteins. This basement membrane, roughly at mid-plane in an alveolar septum, has a width of about $0.5 \mu\text{m}$ [17]. Inertial forces generated by these membranes are to be based upon a membrane thickness of $\sim 5 \mu\text{m}$ with an approximate density of water, while the structural forces that they carry are to be based upon a basement membrane thickness of $\sim 0.5 \mu\text{m}$.

It is not known how much of the mechanical load is actually carried by the cells in an alveolar septum vs. the extracellular basement membrane they encase, but it is generally thought that this basement membrane carries the majority of the load [62]. Therefore, by diminishing the moduli that are appropriate for describing a basement membrane with thickness $\sim 0.5 \mu\text{m}$ by a factor of 10, we get estimates for effective septal moduli that are applicable when modeling a whole septal membrane with thickness $\sim 5 \mu\text{m}$. We use the model parameters obtained for a visceral pleura membrane [51] and the above conjecture to model alveolar septa, as specified in Table 4.3.

Collagen and elastin appear as thin filaments randomly oriented and somewhat uniformly dispersed throughout a basement membrane, unlike the strongly aligned fibers that appear in septal chords. Consequently, for our purposes, we model this collective ensemble of tissue and structure types as a homogeneous isotropic membrane modeled after the Freed-Rajagopal biologic fiber [90] that we have extended to membranes in Appendix A, specifically

$$\frac{1}{M} = \frac{\xi_t - \xi_1}{M_1 \xi_t + s^\pi/2} + \frac{1}{M_2} \quad \xi_1 = \xi - \alpha(\theta - \theta_0) - \frac{s^\pi}{4M_2} \quad (4.26a)$$

$$\frac{1}{G} = \Gamma \left(\frac{\gamma_t - 2\varepsilon\gamma - |\gamma_1|}{G_1 \gamma_t + 2\varepsilon s^\tau} + \frac{1 - 2\varepsilon}{G_2} \right) \quad \gamma_1 = \gamma - \frac{(1 - 2\varepsilon)s^\tau}{G_2} \quad (4.26b)$$

where the compliant tangent moduli of M_1 and G_1 and the stiff, terminal, tangent moduli of M_2 and G_2 bound their responses in that $M_1 \leq M \leq M_2$ and $G_1 \leq G \leq G_2$, with gradual transitions between their asymptotic bounds being centered around strains of ξ_t and γ_t .

Property	Value
ρ [gr/cm ³]	1.1
η_0 [erg/gr.K]	5.0×10^6
C [erg/gr.K]	2.1×10^7
α [1/C]	1.2×10^{-4}
ξ_t	0.24
M_1 [barye]	8.0×10^2
M_2 [barye]	2.2×10^5
γ_t	0.4
G_1 [barye]	5.0×10^2
G_2 [barye]	1.5×10^4

Table 4.3: The elastic properties are for visceral pleura taken from [51], divided by 10 to adjust for septal thickness vs. basement membrane thickness. The thermophysical properties lie between that of water and collagen, weighted towards that of water and evaluated at body temperature.

Finite element technology is used to interpolate the entropy and these stresses, integrated at the Gauss points, to entropies and forces at the vertices of a pentagon, cf. Part 6. The actual entropies and forces interpolated to these nodes are halved, because each septal plane belongs to two adjoining alveoli.

4.4.4. Modeling an Alveolar Volume Subjected to Shock Waves

Alveoli are connected to bronchial trees via alveolar ducts. Under normal conditions, air moves in and out of the alveoli via these ducts. However, when subjected to a stress wave passing over an alveolus, there is no time for the transport of air to take place. Hence, we can consider the air (and heat) within an alveolus to become ‘trapped’, and the pressure to be uniform therein. The governing process is therefore adiabatic. It is under this condition that we model the volumetric response of an alveolar sac.

4.4.4.1. Alveoli Filled with Air

Considering the saturated air within an alveolus to be an ideal gas, then [91]

$$PV = nR\theta \quad \text{or} \quad \frac{PV}{\theta} = \frac{P_0V_0}{\theta_0} = nR = \text{constant} \quad (4.27)$$

where, in our case, P_0 is taken to be atmospheric pressure at sea level (1 bar or 10^5 Pa or 10^6 barye), with V_0 being that alveolar volume whereat alveolar pressure and plural pressure are both atmospheric, while $\theta_0 = 37^\circ\text{C} = 310\text{ K}$ is assigned as body temperature. Parameter n is the molar content of gas within an alveolus, and R is the universal gas constant.

The material constants associated with an ideal gas contained within an adiabatic enclosure are

$$\alpha := \frac{1}{L} \left. \frac{\partial L}{\partial \theta} \right|_P = \frac{1}{3V} \left. \frac{\partial V}{\partial \theta} \right|_P = \frac{1}{3\theta_0} \frac{P_0V_0}{PV} \quad \text{and} \quad K := -V \left. \frac{\partial P}{\partial V} \right|_\theta = P_0 \frac{V_0\theta}{\theta_0 V} \quad (4.28)$$

with the other two material constants pertaining to moist air at body temperature⁹ being its mass density ρ of 1.125×10^{-3} gr/cm³ and its specific heat C of 1.007×10^7 erg/gr.K at constant pressure, constrained by the fact that $K < K_{\max} = \rho C / \alpha^2 \theta \approx \rho C \theta$. An alveolar sac, when modeled as an adiabatic pressure vessel filled with an ideal gas, is described by

$$\begin{Bmatrix} d\eta \\ -3dP \end{Bmatrix} = \begin{bmatrix} C/\theta - 9\alpha^2 K/\rho & 9\alpha K/\rho \\ -9\alpha K & 9K \end{bmatrix} \begin{Bmatrix} d\theta \\ d\Xi \end{Bmatrix} \quad (4.9c)$$

where the entropy within an alveolar sac is given by $S^a = \rho V \eta$ whose initial condition is $S_0^a = \rho V_0 \eta_0$ with $\rho \eta_0$ being the entropy per unit volume of humid air at body temperature and atmospheric pressure, viz., $\rho \eta_0 = 7.770 \times 10^4$ erg/cm³.K. Equation (4.9c) in conjunction with the physical parameters describing an ideal gas (4.28) result in the following equation governing pressure

$$\frac{dP}{P} = \frac{P_0 V_0 \theta}{P V \theta_0} \left(\frac{P_0 V_0 \theta}{P V \theta_0} \frac{d\theta}{\theta} - \frac{dV}{V} \right)$$

where pressure, volume and temperature all appear as logarithmic rates.

Pressure P is mapped to nodal forces at the vertices of a dodecahedron in our alveolar model. This requires finite element technology, which is discussed in Part 6.

4.4.4.2. Alveoli Filled with Fluid

In lung tissues that are not healthy, fluids may fill alveolar volumes at various regions within a lung, e.g., as could be caused by injury, pneumonia, etc. In such localities the mechanical response of the local parenchyma will be vastly stiffer than that of healthy tissue, and as such, it will respond very differently to a traveling shock wave.

In the presence of a passing shock wave, we conjecture that an unhealthy alveolar sac, like a healthy one, can be modeled as an adiabatic enclosure, but now the fluid within such an alveolus is considered to behave, momentarily, like an elastic solid.

The thermoelastic response of an alveolar volume, as described in Eqn. (4.22), is governed by three sets of uncoupled differential equations. The first set of ODEs establishes the uniform response of Eqn. (4.22a) described by

$$\begin{Bmatrix} d\eta \\ d\Pi \end{Bmatrix} = \begin{bmatrix} C/\theta - 3\alpha^2 K/\rho & 3\alpha K/\rho \\ -3\alpha K & 9K \end{bmatrix} \begin{Bmatrix} d\theta \\ d\Xi \end{Bmatrix} \quad \text{where } K = K(\theta, \Pi, \Xi)$$

with the second set of ODEs in Eqn. (4.22b) governing the squeeze response

$$\begin{Bmatrix} d\sigma_1 \\ d\sigma_2 \end{Bmatrix} = \frac{3}{2} \begin{bmatrix} 2N_1 & -N_2 \\ -N_1 & 2N_2 \end{bmatrix} \begin{Bmatrix} d\varepsilon_1 \\ d\varepsilon_2 \end{Bmatrix} \quad \text{where } \begin{aligned} N_1 &= N(\sigma_1, \varepsilon_1) \\ N_2 &= N(\sigma_2, \varepsilon_2) \end{aligned}$$

while the third set of ODEs in Eqn. (4.22c) governs the shear response

$$\begin{Bmatrix} d\tau_1 \\ d\tau_2 \\ d\tau_3 \end{Bmatrix} = \begin{bmatrix} G_1 & 0 & 0 \\ 0 & G_2 & 0 \\ 0 & 0 & G_3 \end{bmatrix} \begin{Bmatrix} d\gamma_1 \\ d\gamma_2 \\ d\gamma_3 \end{Bmatrix} \quad \text{where } \begin{aligned} G_1 &= G(\tau_1, \gamma_1) \\ G_2 &= G(\tau_2, \gamma_2) \\ G_3 &= G(\tau_3, \gamma_3) \end{aligned}$$

⁹The physical properties listed for air were taken from the website www.peacesoftware.de hosted by Berndt Wischnewski.

that collectively can be used to describe the thermoelastic response of a volume of material.

How these are to be parameterized will be addressed in next year's work.

4.5. Finite Element Implementation of Constitutive Equations

These constitutive models are implemented into our finite element model as hypo-elastic material models [66] described by¹⁰

$$d\boldsymbol{\sigma} = \mathbf{M}(\boldsymbol{\sigma}, \boldsymbol{\epsilon}) d\boldsymbol{\epsilon} \quad \text{wherein} \quad d\boldsymbol{\epsilon} = \frac{d\boldsymbol{\varepsilon}(\boldsymbol{\lambda})}{d\boldsymbol{\lambda}} d\boldsymbol{\lambda} \quad (4.29)$$

where $\boldsymbol{\sigma}$, $\boldsymbol{\epsilon}$ and $\boldsymbol{\lambda}$ are arrays of stress, strain and stretch attributes, respectively, with matrix $\mathbf{M}(\boldsymbol{\sigma}, \boldsymbol{\epsilon})$ containing the constitutive tangent moduli, i.e., $d\boldsymbol{\sigma}/d\boldsymbol{\epsilon}$, that, in general, may depend upon both stress $\boldsymbol{\sigma}$ and strain $\boldsymbol{\epsilon}$, while strain depends solely upon stretch $\boldsymbol{\lambda}$.

The two-step PECE algorithm presented in §5.1.1 presumes the following information. There is an initial condition for the thermodynamic stresses $\boldsymbol{\sigma}_0$. An initial far-field deformation gradient \mathbf{F}_0 is also known, from which initial conditions for the thermodynamic stretches $\boldsymbol{\lambda}_0$ and strains $\boldsymbol{\epsilon}_0$ are readily obtained. All nodes of integration are to be spaced uniformly in time with $h > 0$ designating their separation in time.

A far-field deformation gradient is considered to be known at the end of the first integration step, i.e., \mathbf{F}_1 , from which the thermodynamic stretches $\boldsymbol{\lambda}_1$ and strains $\boldsymbol{\epsilon}_1$ are readily calculated, with differential rates $d\boldsymbol{\lambda}_0$ and $d\boldsymbol{\lambda}_1$ coming from finite difference formulæ, from which $d\boldsymbol{\epsilon}_0 = [d\boldsymbol{\varepsilon}(\boldsymbol{\lambda}_0)/d\boldsymbol{\lambda}_0] d\boldsymbol{\lambda}_0$ and $d\boldsymbol{\epsilon}_1 = [d\boldsymbol{\varepsilon}(\boldsymbol{\lambda}_1)/d\boldsymbol{\lambda}_1] d\boldsymbol{\lambda}_1$ follow. Consequently, an initial stress rate can be established, i.e., $d\boldsymbol{\sigma}_0 = \mathbf{M}(\boldsymbol{\sigma}_0, \boldsymbol{\epsilon}_0) d\boldsymbol{\epsilon}_0$. With this information, Heun's method (Eqn. 5.1) can be called upon to integrate Eqn. (4.29) to determine the thermodynamic stresses and their differential rates out to the end of the first integration step, viz., $\boldsymbol{\sigma}_1$ after which one can determine $d\boldsymbol{\sigma}_1 = \mathbf{M}(\boldsymbol{\sigma}_1, \boldsymbol{\epsilon}_1) d\boldsymbol{\epsilon}_1$.

For the next step, and those that follow, the more stable two-step method of Eqn. (5.2) can be called upon to advance a solution for the thermodynamic stresses and their differential rates. What needs to be stored are variables from the previous step, viz., $\boldsymbol{\sigma}_{n-1}$, $\boldsymbol{\lambda}_{n-1}$ and $d\boldsymbol{\sigma}_{n-1}$, along with like variables from the current step, viz., $\boldsymbol{\sigma}_n$, $\boldsymbol{\lambda}_n$ and $d\boldsymbol{\sigma}_n$. Then, given a far-field deformation gradient for the next step, i.e., \mathbf{F}_{n+1} , one can determine $\boldsymbol{\lambda}_{n+1}$ and $\boldsymbol{\epsilon}_{n+1}$ along with the differential rate $d\boldsymbol{\lambda}_{n+1}$ obtained from finite difference formulæ, after which $d\boldsymbol{\epsilon}_{n+1} = [d\boldsymbol{\varepsilon}(\boldsymbol{\lambda}_{n+1})/d\boldsymbol{\lambda}_{n+1}] d\boldsymbol{\lambda}_{n+1}$ can be established. With this information, the PECE method (Eqn. 5.2) can be called upon to integrate Eqn. (4.29) to determine the thermodynamic stresses and their differential rates out to the end of the next integration step, viz., $\boldsymbol{\sigma}_{n+1}$ along with $d\boldsymbol{\sigma}_{n+1} = \mathbf{M}(\boldsymbol{\sigma}_{n+1}, \boldsymbol{\epsilon}_{n+1}) d\boldsymbol{\epsilon}_{n+1}$.

¹⁰Constitutive equation $d\boldsymbol{\sigma} = \mathbf{M}(\boldsymbol{\sigma}, \boldsymbol{\epsilon}) d\boldsymbol{\epsilon}$ is that of a hypo-elastic solid [66]. A reasonable viscoelastic constitutive equation that one could consider would be a Zener [92] solid, which would look something like

$$\boldsymbol{\sigma} + \boldsymbol{\tau} d\boldsymbol{\sigma} = \mathbf{E}_\infty \boldsymbol{\epsilon} + \boldsymbol{\tau} \mathbf{E}_0 d\boldsymbol{\epsilon}$$

where \mathbf{E}_∞ is a matrix of rubbery moduli, \mathbf{E}_0 is a matrix of glassy moduli, and $\boldsymbol{\tau}$ is a matrix of characteristic relaxation times. This is a topic for future work.

4.5.1. 1D Formulation

For any given alveolar chord, we know its reference length L_0 and its current length L from which chordal stretch is described by $\lambda := L/L_0$ and its strain is defined as $e := \ln \lambda$ whose differential rate of change is $de = L^{-1} dL$; consequently,

$$\begin{Bmatrix} d\theta \\ de \end{Bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1/L \end{bmatrix} \begin{Bmatrix} d\theta \\ dL \end{Bmatrix} \quad (4.30)$$

where the matrix establishes $d\varepsilon(\boldsymbol{\lambda})/d\boldsymbol{\lambda}$ in Eqn. (4.29) for a chord, with $d\boldsymbol{\lambda}$ being the vector to the right of this matrix, and $d\varepsilon$ being the vector on the left-hand side. Finite difference formulæ are used to quantify $d\theta$ and dL .

The matrix of tangent moduli $\mathbf{M}(\boldsymbol{\sigma}, \varepsilon)$ given in Eqn. (4.29) is Eqn. (4.9a) for the case of a chord, whose elastic modulus is $E(\theta, s, e)$ with stress defined as $s := F/A = \lambda F/A_0$, where F is the force carried by the chord, and where A_0 and A are the chordal cross-sectional areas in its reference and current states, respectively. Here it is assumed that chordal volume is preserved, which is a reasonable assumption for soft biological structures. The vector being operated on by this matrix of tangent moduli is $d\varepsilon$ above, with the constitutive equation returning a vector $d\boldsymbol{\sigma} = \{d\eta, ds\}^\top$. The numerical method presented in §5.1.1 can then be called upon to integrate this hypo-elastic constitutive equation for its thermodynamic stresses $\boldsymbol{\sigma}$.

4.5.2. 2D Formulation

Consider an incoming deformation gradient $\mathbf{F} = \mathcal{F}_{ij} \vec{\mathbf{e}}_i \otimes \vec{\mathbf{e}}_j$, $i, j = 1, 2$, whose components \mathcal{F}_{ij} are evaluated in a co-ordinate system associated with a membrane whose base vectors $(\vec{\mathbf{e}}_1, \vec{\mathbf{e}}_2)$, cf. Fig. 2.5, have been re-indexed via an orthogonal matrix \mathbf{P} according to §3.3.5.3. It is in this co-ordinate system that the components of Laplace stretch $\mathbf{U} = \mathcal{U}_{ij} \vec{\mathbf{e}}_i \otimes \vec{\mathbf{e}}_j$ and its inverse \mathbf{U}^{-1} are quantified via

$$\mathbf{U} = \begin{bmatrix} a & ag \\ 0 & b \end{bmatrix}, \quad \mathbf{U}^{-1} = \begin{bmatrix} 1/a & -g/b \\ 0 & 1/b \end{bmatrix} \quad \text{with} \quad \begin{aligned} \mathcal{U}_{11} &= \sqrt{\mathcal{C}_{11}} & \mathcal{U}_{12} &= \mathcal{C}_{12}/\mathcal{U}_{11} \\ \mathcal{U}_{21} &= 0 & \mathcal{U}_{22} &= \sqrt{\mathcal{C}_{22} - \mathcal{U}_{12}^2} \end{aligned} \quad (4.31)$$

whose physical attributes for stretch are then defined by

$$a := \mathcal{U}_{11} > 0, \quad b := \mathcal{U}_{22} > 0, \quad g := \frac{\mathcal{U}_{12}}{\mathcal{U}_{11}} \quad (4.32)$$

wherein $\mathbf{C} = \mathbf{F}^\top \mathbf{F}$ denotes the right Cauchy-Green deformation tensor $\mathbf{C} = \mathcal{C}_{ij} \vec{\mathbf{e}}_i \otimes \vec{\mathbf{e}}_j$ that is affiliated with a membrane whose components $\mathcal{C}_{ij} = \mathcal{F}_{ki} \mathcal{F}_{kj}$ are evaluated in basis $(\vec{\mathbf{e}}_1, \vec{\mathbf{e}}_2)$.

Given a sequence of deformation gradients spaced at uniform time intervals of h , one can construct differential rates for the stretch attributes via finite difference formulæ [39]. Specifically, from the forward difference formula $\dot{\mathcal{U}}_0 = (\mathcal{U}_1 - \mathcal{U}_0)/h + \mathcal{O}(h)$ one finds that

$$da_0 = \frac{a_1 - a_0}{h}, \quad db_0 = \frac{b_1 - b_0}{h}, \quad dg_0 = \frac{a_1}{a_0} \left(\frac{g_1 - g_0}{h} \right) \quad (4.33a)$$

while from the backward difference formula $\dot{\mathcal{U}}_1 = (\mathcal{U}_1 - \mathcal{U}_0)/h + \mathcal{O}(h)$ one gets

$$da_1 = \frac{a_1 - a_0}{h}, \quad db_1 = \frac{b_1 - b_0}{h}, \quad dg_1 = \frac{a_0}{a_1} \left(\frac{g_1 - g_0}{h} \right) \quad (4.33b)$$

where the finite difference formulæ for states ‘0’ and ‘1’ are first-order accurate. A second-order accurate, backward, difference formula $\dot{\mathcal{U}}_{n+1} = (3\mathcal{U}_{n+1} - 4\mathcal{U}_n + \mathcal{U}_{n-1})/2h + \mathcal{O}(h^2)$, $n = 1, 2, \dots, N$, can be used for states ‘2’ and onward, from which one determines that

$$\begin{aligned} da_{n+1} &= \frac{3a_{n+1} - 3a_n + a_{n-1}}{2h} \\ db_{n+1} &= \frac{3b_{n+1} - 2b_n + b_{n-1}}{2h} \\ dg_{n+1} &= 2 \frac{a_n}{a_{n+1}} \left(\frac{g_{n+1} - g_n}{h} \right) - \frac{a_{n-1}}{a_{n+1}} \left(\frac{g_{n+1} - g_{n-1}}{2h} \right). \end{aligned} \quad (4.33c)$$

The associated thermodynamic strains and their differential rates at the n^{th} step are then quantified via

$$\xi_n = \ln \left(\sqrt{\frac{a_n}{a_0} \frac{b_n}{b_0}} \right) \quad d\xi_n = \frac{1}{2} \left(\frac{da_n}{a_n} + \frac{db_n}{b_n} \right) \quad (4.34a)$$

$$\varepsilon_n = \ln \left(\sqrt{\frac{a_n}{a_0} \frac{b_0}{b_n}} \right) \quad d\varepsilon_n = \frac{1}{2} \left(\frac{da_n}{a_n} - \frac{db_n}{b_n} \right) \quad (4.34b)$$

$$\gamma_n = g_n - g_0 \quad d\gamma_n = dg_n \quad (4.34c)$$

where $n = 0, 1, 2, \dots, N$. This supposes initial conditions of $\xi_0 = \varepsilon_0 = \gamma_0 = 0$. Differential rates of the physical attributes relate to differential rates of the thermodynamic variables according to

$$\begin{Bmatrix} d\theta \\ d\xi \\ d\varepsilon \\ d\gamma \end{Bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/2a & 1/2b & 0 \\ 0 & 1/2a & -1/2b & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} da \\ db \\ dg \end{Bmatrix} \quad (4.35)$$

where the above matrix establishes $d\boldsymbol{\varepsilon}(\boldsymbol{\lambda})/d\boldsymbol{\lambda}$ in Eqn. (4.29) for a membrane, with $d\boldsymbol{\lambda}$ being the vector to the right of this matrix, and $d\boldsymbol{\varepsilon}$ being the vector on the left-hand side.

The matrix of tangent moduli $\mathbf{M}(\boldsymbol{\sigma}, \boldsymbol{\varepsilon})$ given in Eqn. (4.29) is Eqn. (4.15) for the case of a membrane, whose moduli are: an areal modulus $M(\theta, \pi, \xi)$, a squeeze modulus $N(\sigma, \varepsilon)$, and a shear modulus $G(\tau, \gamma)$. The vector being operated on by this matrix of tangent moduli is $d\boldsymbol{\varepsilon}$ above, with the constitutive equation returning a vector $d\boldsymbol{\sigma} = \{d\eta, d\pi, d\sigma, d\tau\}^\top$. The numerical method presented in §5.1.1 can then be called upon to integrate this hypo-elastic constitutive equation for its thermodynamic stresses $\boldsymbol{\sigma}$.

After this constitutive equation has been integrated, the ensuing thermodynamic stress attributes can be mapped into components \mathcal{S}_{ij} of a stress tensor $\boldsymbol{\mathcal{S}} = \mathcal{S}_{ij} \vec{\mathbf{e}}_i \otimes \vec{\mathbf{e}}_j$, $i, j = 1, 2$,

evaluated in the basis $(\vec{\mathbf{e}}_1, \vec{\mathbf{e}}_2)$ of a membrane; specifically,

$$\begin{Bmatrix} \eta \\ \mathcal{S}_{11} \\ \mathcal{S}_{22} \\ \mathcal{S}_{12} = \mathcal{S}_{21} \end{Bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/2 & 1/2 & 0 \\ 0 & 1/2 & -1/2 & 0 \\ 0 & 0 & 0 & b/a \end{bmatrix} \begin{Bmatrix} \eta \\ \pi \\ \sigma \\ \tau \end{Bmatrix}. \quad (4.36)$$

These physical stress components \mathcal{S}_{ij} can be pulled back into components S_{ij} belonging to the Lagrangian, second, Piola-Kirchhoff stress $\mathbf{S} = S_{ij} \vec{\mathbf{e}}_i \otimes \vec{\mathbf{e}}_j$ or rotated into components s_{ij} belonging to the Eulerian Kirchhoff stress $\mathbf{s} = s_{ij} \vec{\mathbf{e}}_i \otimes \vec{\mathbf{e}}_j$ via

$$S_{ij} = \mathcal{U}_{ik}^{-1} \mathcal{S}_{k\ell} \mathcal{U}_{j\ell}^{-1} \quad \text{or} \quad s_{ij} = \mathcal{F}_{ik} S_{k\ell} \mathcal{F}_{j\ell} = \mathcal{R}_{ik} \mathcal{S}_{k\ell} \mathcal{R}_{j\ell} \quad (4.37)$$

where $\mathcal{R} = \mathbf{F}\mathcal{U}^{-1}$ is the Gram rotation that associates with Laplace stretch, viz., $\mathbf{F} = \mathcal{R}\mathbf{U}$.

Components S_{ij} belonging to the Lagrangian, second, Piola-Kirchhoff stress \mathbf{S} and components s_{ij} belonging to the Eulerian Kirchhoff stress \mathbf{s} , as established in Eqn. (4.37), are evaluated in a re-indexed co-ordinate system with base vectors $(\vec{\mathbf{e}}_1, \vec{\mathbf{e}}_2)$. To map these components back into the co-ordinate system of the ‘user’, one must apply the linear transformations

$$P_{ik} S_{k\ell} P_{j\ell} \quad \text{and} \quad P_{ik} s_{k\ell} P_{j\ell}$$

where \mathbf{P} is the orthogonal matrix defined in Eqn. (3.24).

4.5.3. 3D Formulation

From an incoming deformation gradient $\mathbf{F} = \mathcal{F}_{ij} \vec{\mathbf{E}}_i \otimes \vec{\mathbf{E}}_j$, $i, j = 1, 2, 3$, whose components \mathcal{F}_{ij} are evaluated in a re-indexed co-ordinate system with base vectors $(\vec{\mathbf{E}}_1, \vec{\mathbf{E}}_2, \vec{\mathbf{E}}_3)$, as established in §2.1, it follows that the components for Laplace stretch $\mathcal{U} = \mathcal{U}_{ij} \vec{\mathbf{E}}_i \otimes \vec{\mathbf{E}}_j$ and its inverse \mathcal{U}^{-1} are given by

$$\mathcal{U} = \begin{bmatrix} a & a\gamma & a\beta \\ 0 & b & b\alpha \\ 0 & 0 & c \end{bmatrix} \quad \text{and} \quad \mathcal{U}^{-1} = \begin{bmatrix} 1/a & -\gamma/b & -(\beta - \alpha\gamma)/c \\ 0 & 1/b & -\alpha/c \\ 0 & 0 & 1/c \end{bmatrix} \quad (4.38)$$

where components \mathcal{U}_{ij} are evaluated according to formulæ

$$\begin{aligned} \mathcal{U}_{11} &= \sqrt{\mathcal{C}_{11}} & \mathcal{U}_{12} &= \mathcal{C}_{12}/\mathcal{U}_{11} & \mathcal{U}_{13} &= \mathcal{C}_{13}/\mathcal{U}_{11} \\ \mathcal{U}_{21} &= 0 & \mathcal{U}_{22} &= \sqrt{\mathcal{C}_{22} - \mathcal{U}_{12}^2} & \mathcal{U}_{23} &= (\mathcal{C}_{23} - \mathcal{U}_{12}\mathcal{U}_{13})/\mathcal{U}_{22} \\ \mathcal{U}_{31} &= 0 & \mathcal{U}_{32} &= 0 & \mathcal{U}_{33} &= \sqrt{\mathcal{C}_{33} - \mathcal{U}_{13}^2 - \mathcal{U}_{23}^2} \end{aligned} \quad (4.39)$$

thereby permitting their physical attributes for stretch to be established as

$$a := \mathcal{U}_{11} > 0, \quad b := \mathcal{U}_{22} > 0, \quad c := \mathcal{U}_{33} > 0, \quad \alpha := \frac{\mathcal{U}_{23}}{\mathcal{U}_{22}}, \quad \beta := \frac{\mathcal{U}_{13}}{\mathcal{U}_{11}}, \quad \gamma := \frac{\mathcal{U}_{12}}{\mathcal{U}_{11}} \quad (4.40)$$

wherein $\mathbf{C} = \mathbf{F}^\top \mathbf{F} = \mathcal{C}_{ij} \vec{\mathbf{E}}_i \otimes \vec{\mathbf{E}}_j$ is the right Cauchy-Green deformation tensor with components $\mathcal{C}_{ij} = \mathcal{F}_{ki} \mathcal{F}_{kj}$. The stretch attributes a, b and c are elongation ratios, while the remaining stretch attributes α, β and γ are the magnitudes of shear, cf. §3.4.2.

Given a sequence of deformation gradients spaced at uniform time intervals of h , one can construct differential rates for the stretch attributes via finite difference formulæ [39]. Specifically, from the forward difference formula $\dot{\mathbf{U}}_0 = (\mathbf{U}_1 - \mathbf{U}_0)/h + \mathcal{O}(h)$ one finds that

$$\begin{aligned} da_0 &= \frac{a_1 - a_0}{h} & d\alpha_0 &= \frac{b_1}{b_0} \left(\frac{\alpha_1 - \alpha_0}{h} \right) \\ db_0 &= \frac{b_1 - b_0}{h} & d\beta_0 &= \frac{a_1}{a_0} \left(\frac{\beta_1 - \beta_0}{h} \right) \\ dc_0 &= \frac{c_1 - c_0}{h} & d\gamma_0 &= \frac{a_1}{a_0} \left(\frac{\gamma_1 - \gamma_0}{h} \right) \end{aligned} \quad (4.41a)$$

while from the backward difference formula $\dot{\mathbf{U}}_1 = (\mathbf{U}_1 - \mathbf{U}_0)/h + \mathcal{O}(h)$ one gets

$$\begin{aligned} da_1 &= \frac{a_1 - a_0}{h} & d\alpha_1 &= \frac{b_0}{b_1} \left(\frac{\alpha_1 - \alpha_0}{h} \right) \\ db_1 &= \frac{b_1 - b_0}{h} & d\beta_1 &= \frac{a_0}{a_1} \left(\frac{\beta_1 - \beta_0}{h} \right) \\ dc_1 &= \frac{c_1 - c_0}{h} & d\gamma_1 &= \frac{a_0}{a_1} \left(\frac{\gamma_1 - \gamma_0}{h} \right) \end{aligned} \quad (4.41b)$$

where the finite difference formulæ for states ‘0’ and ‘1’ are first-order accurate. A second-order accurate, backward difference formula $\dot{\mathbf{U}}_{n+1} = (3\mathbf{U}_{n+1} - 4\mathbf{U}_n + \mathbf{U}_{n-1})/2h + \mathcal{O}(h^2)$, $n = 1, 2, \dots, N$, can be used for states ‘2’ and onward, from which one determines that

$$\begin{aligned} da_{n+1} &= \frac{3a_{n+1} - 4a_n + a_{n-1}}{2h} \\ db_{n+1} &= \frac{3b_{n+1} - 4b_n + b_{n-1}}{2h} \\ dc_{n+1} &= \frac{3c_{n+1} - 4c_n + c_{n-1}}{2h} \\ d\alpha_{n+1} &= \frac{2b_n}{b_{n+1}} \left(\frac{\alpha_{n+1} - \alpha_n}{h} \right) - \frac{b_{n-1}}{b_{n+1}} \left(\frac{\alpha_{n+1} - \alpha_{n-1}}{2h} \right) \\ d\beta_{n+1} &= \frac{2a_n}{a_{n+1}} \left(\frac{\beta_{n+1} - \beta_n}{h} \right) - \frac{a_{n-1}}{a_{n+1}} \left(\frac{\beta_{n+1} - \beta_{n-1}}{2h} \right) \\ d\gamma_{n+1} &= \frac{2a_n}{a_{n+1}} \left(\frac{\gamma_{n+1} - \gamma_n}{h} \right) - \frac{a_{n-1}}{a_{n+1}} \left(\frac{\gamma_{n+1} - \gamma_{n-1}}{2h} \right). \end{aligned} \quad (4.41c)$$

The associated thermodynamic strains and their differential rates at the n^{th} step have an uniform contribution of

$$\Xi_n = \ln \left(\sqrt[3]{\frac{a_n}{a_0} \frac{b_n}{b_0} \frac{c_n}{c_0}} \right) \quad d\Xi_n = \frac{1}{3} \left(\frac{da_n}{a_n} + \frac{db_n}{b_n} + \frac{dc_n}{c_n} \right) \quad (4.42a)$$

have squeeze contributions of

$$\varepsilon_{1n} = \ln \left(\sqrt[3]{\frac{a_n}{a_0} \frac{b_0}{b_n}} \right) \quad d\varepsilon_{1n} = \frac{1}{3} \left(\frac{da_n}{a_n} - \frac{db_n}{b_n} \right) \quad (4.42b)$$

$$\varepsilon_{2n} = \ln \left(\sqrt[3]{\frac{b_n}{b_0} \frac{c_0}{c_n}} \right) \quad d\varepsilon_{2n} = \frac{1}{3} \left(\frac{db_n}{b_n} - \frac{dc_n}{c_n} \right) \quad (4.42c)$$

and have shear contributions of

$$\gamma_{1n} = \alpha_n - \alpha_0 \quad d\gamma_{1n} = d\alpha_n \quad (4.42d)$$

$$\gamma_{2n} = \beta_n - \beta_0 \quad d\gamma_{2n} = d\beta_n \quad (4.42e)$$

$$\gamma_{3n} = \gamma_n - \gamma_0 \quad d\gamma_{3n} = d\gamma_n \quad (4.42f)$$

where $n = 0, 1, 2, \dots, N$. These suppose initial conditions of $\Xi_0 = \varepsilon_{10} = \varepsilon_{20} = \gamma_{10} = \gamma_{20} = \gamma_{30} = 0$. Differential rates of the physical attributes relate to differential rates of the thermodynamic variables according to

$$\begin{Bmatrix} d\theta \\ d\Xi \\ d\varepsilon_1 \\ d\varepsilon_2 \\ d\gamma_1 \\ d\gamma_2 \\ d\gamma_3 \end{Bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/3a & 1/3b & 1/3c & 0 & 0 & 0 \\ 0 & 1/3a & -1/3b & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/3b & -1/3c & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} d\theta \\ da \\ db \\ dc \\ d\alpha \\ d\beta \\ d\gamma \end{Bmatrix} \quad (4.43)$$

where the above matrix establishes $d\boldsymbol{\varepsilon}(\boldsymbol{\lambda})/d\boldsymbol{\lambda}$ in Eqn. (4.29), with $d\boldsymbol{\lambda}$ being the vector at the right of this matrix, and $d\boldsymbol{\varepsilon}$ being the vector on the left-hand side.

The matrix of tangent moduli $\mathbf{M}(\boldsymbol{\sigma}, \boldsymbol{\varepsilon})$ given in Eqn. (4.29) is Eqn. (4.22) for the general case, whose moduli are: an bulk modulus $K(\theta, \Pi, \Xi)$, two squeeze moduli $N_1 = N(\sigma_1, \varepsilon_1)$ and $N_2 = N(\sigma_2, \varepsilon_2)$, and three shear moduli $G_1 = G(\tau_1, \gamma_1)$, $G_2 = G(\tau_2, \gamma_2)$ and $G_3 = G(\tau_3, \gamma_3)$. The vector being operated on by this matrix of tangent moduli is $d\boldsymbol{\varepsilon}$ above, with the constitutive equation returning a vector $d\boldsymbol{\sigma} = \{d\eta, d\Pi, d\sigma_1, d\sigma_2, d\tau_1, d\tau_2, d\tau_3\}^T$. The numerical method presented in §5.1.1 can be called upon to integrate this hypo-elastic constitutive equation.

After this constitutive equation has been integrated, the ensuing thermodynamic stress attributes can be mapped into components \mathcal{S}_{ij} of a physical stress tensor $\boldsymbol{\sigma} = \mathcal{S}_{ij} \vec{\mathbf{E}}_i \otimes \vec{\mathbf{E}}_j$, $i, j = 1, 2, 3$, evaluated in the re-indexed basis $(\vec{\mathbf{E}}_1, \vec{\mathbf{E}}_2, \vec{\mathbf{E}}_3)$ of our dodecahedron; specifically,

$$\begin{Bmatrix} \eta \\ \mathcal{S}_{11} \\ \mathcal{S}_{22} \\ \mathcal{S}_{33} \\ \mathcal{S}_{23} = \mathcal{S}_{32} \\ \mathcal{S}_{13} = \mathcal{S}_{31} \\ \mathcal{S}_{12} = \mathcal{S}_{21} \end{Bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/3 & 2/3 & 1/3 & 0 & 0 & 0 \\ 0 & 1/3 & -1/3 & 1/3 & 0 & 0 & 0 \\ 0 & 1/3 & -1/3 & -2/3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & c/b & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & c/a & 0 \\ 0 & 0 & 0 & 0 & 0 & ab/a & b/a \end{bmatrix} \begin{Bmatrix} \eta \\ \Pi \\ \sigma_1 \\ \sigma_2 \\ \tau_1 \\ \tau_2 \\ \tau_3 \end{Bmatrix}. \quad (4.44)$$

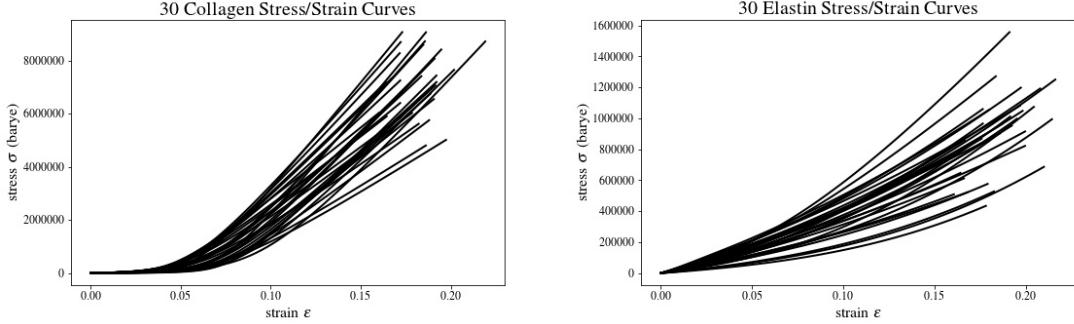


Figure 4.2: Typical stress/strain curves for collagen (left) and elastin (right) fibers that make up a septal chord. Their material parameters have been assigned via statistical distributions.

Collagen		Elastin	
E_1^c [barye]	$5.0 \times 10^5 \pm 2.0 \times 10^5$	E_1^e [barye]	$2.3 \times 10^6 \pm 1.0 \times 10^6$
E_2^c [barye]	$5.0 \times 10^7 \pm 1.0 \times 10^7$	E_2^e [barye]	$1.0 \times 10^7 \pm 2.0 \times 10^6$
e_t^c	0.09 ± 0.015	e_t^e	0.4 ± 0.1

Table 4.4: Physical properties for hydrated collagen and elastin fibers when described with the fiber model of Freed & Rajagopal [90].

These physical components S_{ij} can be pulled back into components S_{ij} belonging to the Lagrangian, second, Piola-Kirchhoff stress $\mathbf{S} = S_{ij} \vec{\mathbf{E}}_i \otimes \vec{\mathbf{E}}_j$ or rotated into components s_{ij} belonging to the Eulerian Kirchhoff stress $\mathbf{s} = s_{ij} \vec{\mathbf{E}}_i \otimes \vec{\mathbf{E}}_j$ via

$$S_{ij} = \mathcal{U}_{ik}^{-1} \mathcal{S}_{kl} \mathcal{U}_{jl}^{-1} \quad \text{or} \quad s_{ij} = \mathcal{F}_{ik} S_{kl} \mathcal{F}_{jl} = \mathcal{R}_{ik} \mathcal{S}_{kl} \mathcal{R}_{jl} \quad (4.45)$$

where $\mathcal{R} = \mathbf{F}\mathcal{U}^{-1}$ is the Gram rotation that associates with Laplace stretch, viz., $\mathbf{F} = \mathcal{R}\mathcal{U}$.

Components S_{ij} belonging to the Lagrangian, second, Piola-Kirchhoff stress \mathbf{S} and components s_{ij} belonging to the Eulerian Kirchhoff stress \mathbf{s} , as established in Eqn. (4.37), are evaluated in a re-indexed co-ordinate system with base vectors $(\vec{\mathbf{E}}_1, \vec{\mathbf{E}}_2, \vec{\mathbf{E}}_3)$. To map these components back into the co-ordinate system of the ‘user’ one must apply the linear transformations

$$P_{ik} S_{kl} P_{jl} \quad \text{and} \quad P_{ik} s_{kl} P_{jl}$$

where \mathbf{P} is the orthogonal matrix defined in §2.1.

4.6. Code Verification and Constitutive Parameterization

All material parameters are assigned from their respective statistical distributions. For example, there are thirty chords in a dodecahedron comprised of collagen and elastin fibers that are loaded in parallel. Figure 4.2 presents a typical set of stress/strain response curves for the chords of a dodecahedron whose parameters are displayed in Table 4.4.

Recently, Birzle *et al.* [63] performed experiments on thin slices of rat parenchyma loaded in tension where they removed the collagen and/or elastin fiber through collagenase and elastase baths to study their individual behaviors and their interactions under load.

Part 5

Numerical Integrators

This analysis tool, which models the geometry of alveoli as a dodecahedron, requires numerical methods to integrate the constitutive equations (systems of first-order ODEs), the governing equations of motion (systems of second-order ODEs), and that integrate the length, area or volume of the finite elements (handled using Gaussian quadrature). The numerical methods used in this work are discussed below.

5.1. ODE Solvers

The various constitutive equations that describe our alveolar model present themselves as ordinary differential equations that need to be integrated. To this end, we employ the PECE (Predict, Evaluate, Correct, re-Evaluate) algorithms of Freed [93] which are suitable for solving stiff systems of first- and second-order, ordinary, differential equations. These methods are based upon Gear's well-known second-order backward difference formula (BDF2, which is Eqns. 5.2c & 5.6e below).

Time t is considered to be the independent variable, discretized over an interval in time $[t_0, t_N]$ for which N solutions are to be extracted at nodes $n = 1, 2, \dots, N$ spaced at uniform intervals in time with a common step size of $h = (t_N - t_0)/N$ separating them, where time t_0 associates with the initial conditions. This is the *global step size* at which solutions are to be gathered. A dynamically controlled *local step size*, whose size is adjusted on the fly via a PI controller to manage truncation error, is implemented into the code according to a scheme put forward in Ref. [94]. Solver interfaces are listed in Appendix H.

5.1.1. PECE Solver for First-Order ODEs

Let \mathbf{x} be a vector of dependent variables obeying a differential equation of evolution $d\mathbf{x}(t)/dt = \dot{\mathbf{x}} = \mathbf{f}(t, \mathbf{x})$ subject to an initial condition $\mathbf{x}_0 = \mathbf{x}(t_0)$ where t is the independent variable, typically time, but not in our case.

The two-step method put forward here incrementally solves such an ODE, returning solutions associated with the next moment in time t_{n+1} , i.e., it acquires \mathbf{x}_{n+1} , given knowledge of the previous \mathbf{x}_{n-1} and current \mathbf{x}_n solutions plus their rates $\dot{\mathbf{x}}_{n-1}$ and $\dot{\mathbf{x}}_n$ with the corrector also depending upon $\dot{\mathbf{x}}_{n+1}$, i.e., the corrector is an implicit method.

5.1.1.1. Start-Up Algorithm

Multi-step methods are not self starting; consequently, Heun's method (a forward-Euler predictor with a trapezoidal corrector) is used here to start our integrator; specifically,

$$\text{Predict} \quad \mathbf{x}_1^p = \mathbf{x}_0 + h\dot{\mathbf{x}}_0 + \mathcal{O}(h^2) \quad (5.1a)$$

$$\text{Evaluate} \quad \dot{\mathbf{x}}_1^p = \mathbf{f}(t_1, \mathbf{x}_1^p) \quad (5.1b)$$

$$\text{Correct} \quad \mathbf{x}_1 = \mathbf{x}_0 + \frac{1}{2}h(\dot{\mathbf{x}}_1^p + \dot{\mathbf{x}}_0) + \mathcal{O}(h^3) \quad (5.1c)$$

$$\text{Re-Evaluate} \quad \dot{\mathbf{x}}_1 = \mathbf{f}(t_1, \mathbf{x}_1) \quad (5.1d)$$

wherein $\dot{\mathbf{x}}_0 = \mathbf{f}(t_0, \mathbf{x}_0)$ and $t_1 = t_0 + h$. The correct/re-evaluate steps can be iterated over until a convergence criterion is satisfied, if need be.

5.1.1.2. Two-Step ODE Solver

The two-step method of Freed [93] for solving 1st order ODEs is

$$\text{Predict} \quad \mathbf{x}_{n+1}^p = \frac{1}{3}(4\mathbf{x}_n - \mathbf{x}_{n-1}) + \frac{2}{3}h(2\dot{\mathbf{x}}_n - \dot{\mathbf{x}}_{n-1}) + \mathcal{O}(h^3) \quad (5.2a)$$

$$\text{Evaluate} \quad \dot{\mathbf{x}}_{n+1}^p = \mathbf{f}(t_{n+1}, \mathbf{x}_{n+1}^p) \quad (5.2b)$$

$$\text{Correct} \quad \mathbf{x}_{n+1} = \frac{1}{3}(4\mathbf{x}_n - \mathbf{x}_{n-1}) + \frac{2}{3}h\dot{\mathbf{x}}_{n+1}^p + \mathcal{O}(h^3) \quad (5.2c)$$

$$\text{Re-Evaluate} \quad \dot{\mathbf{x}}_{n+1} = \mathbf{f}(t_{n+1}, \mathbf{x}_{n+1}) \quad (5.2d)$$

where $t_{n+1} = t_n + h$. This corrector is the well-known BDF2 formula of Gear to which Freed provided a predictor. The correct/re-evaluate steps can be iterated over until a convergence criterion is satisfied, if need be. Implementation of this integrator is found in Appendix H.1.

For both the predictor and corrector, solution \mathbf{x} has a weight of 1, while its rate $\dot{\mathbf{x}}$ has a weight of $\frac{2}{3}h$; hence, this predictor/corrector pair is internally consistent, i.e., the predictor and corrector produce the same result when integrating a constant velocity field.

5.1.2. A Relevant Example

In our finite element implementation, a hypo-elastic material model [66] is introduced to describe the constitutive response of an alveolus whereby

$$\dot{\boldsymbol{\sigma}} = \mathbf{M}(\boldsymbol{\sigma}, \boldsymbol{\epsilon}) \dot{\boldsymbol{\epsilon}} \quad \text{or equivalently [95]} \quad d\boldsymbol{\sigma} = \mathbf{M}(\boldsymbol{\sigma}, \boldsymbol{\epsilon}) d\boldsymbol{\epsilon}$$

where $\boldsymbol{\epsilon}$ is a vector of thermodynamic strains, $\boldsymbol{\sigma}$ is a vector of thermodynamic stresses, and \mathbf{M} is a square matrix comprised of their tangent moduli, which can depend both upon stress and strain. In our application, the thermodynamic stress attributes are

$$\boldsymbol{\sigma}_{1D} = \{\eta, s\}, \quad \boldsymbol{\sigma}_{2D} = \{\eta, s^\pi, s^\sigma, s^\tau\}^\top, \quad \boldsymbol{\sigma}_{3D} = \{\eta, \Pi, \sigma_1, \sigma_2, \tau_1, \tau_2, \tau_3\}^\top$$

where η is entropy and the rest are stresses. Their thermodynamic conjugates are the strain attributes

$$\boldsymbol{\epsilon}_{1D} = \{\theta, e\}, \quad \boldsymbol{\epsilon}_{2D} = \{\theta, \xi, \varepsilon, \gamma\}^\top, \quad \boldsymbol{\epsilon}_{3D} = \{\theta, \Xi, \varepsilon_1, \varepsilon_2, \gamma_1, \gamma_2, \gamma_3\}^\top$$

where θ is temperature and the rest are strains. In the 2- and 3-D cases, these stress-strain attributes arise from Gram-Schmidt decompositions of the deformation gradient (cf. §3.3.5.1, §4.4.3 and §4.5). Constructing tangent moduli $\mathbf{M}(\boldsymbol{\sigma}, \boldsymbol{\epsilon})$ is the topic of Part 4. In the above problem, the thermodynamic strains $\boldsymbol{\epsilon}$ and their differential rates $d\boldsymbol{\epsilon}$ are known, it is their stresses $\boldsymbol{\sigma}$ that must be integrated. Both $\boldsymbol{\sigma}$ and $d\boldsymbol{\sigma} = \mathbf{M} d\boldsymbol{\epsilon}$ arise in the construction of our stiffness matrices, cf. §6.2.

Equation (5.1) is used to take the first step of integration; specifically,

$$\begin{aligned} \text{Predict} \quad & \boldsymbol{\sigma}_1^p = \boldsymbol{\sigma}_0 + h d\boldsymbol{\sigma}_0 \\ \text{Evaluate} \quad & d\boldsymbol{\sigma}_1^p = \mathbf{M}(\boldsymbol{\sigma}_1^p, \boldsymbol{\epsilon}) d\boldsymbol{\epsilon}_1 \\ \text{Correct} \quad & \boldsymbol{\sigma}_1 = \boldsymbol{\sigma}_0 + \frac{1}{2}h(d\boldsymbol{\sigma}_1^p + d\boldsymbol{\sigma}_0) \\ \text{Re-Evaluate} \quad & d\boldsymbol{\sigma}_1 = \mathbf{M}(\boldsymbol{\sigma}_1, \boldsymbol{\epsilon}_1) d\boldsymbol{\epsilon}_1 \end{aligned}$$

where $d\boldsymbol{\sigma}_0 = \mathbf{M}(\boldsymbol{\sigma}_0, \boldsymbol{\epsilon}_0) d\boldsymbol{\epsilon}_0$, with the remaining steps of integration following according to Eqn. (5.2), specifically

Predict	$\boldsymbol{\sigma}_{n+1}^p = \frac{1}{3}(4\boldsymbol{\sigma}_n - \boldsymbol{\sigma}_{n-1}) + \frac{2}{3}h(2d\boldsymbol{\sigma}_n - d\boldsymbol{\sigma}_{n-1})$
Evaluate	$d\boldsymbol{\sigma}_{n+1}^p = \mathbf{M}(\boldsymbol{\sigma}_{n+1}^p, \boldsymbol{\epsilon}_{n+1}) d\boldsymbol{\epsilon}_{n+1}$
Correct	$\boldsymbol{\sigma}_{n+1} = \frac{1}{3}(4\boldsymbol{\sigma}_n - \boldsymbol{\sigma}_{n-1}) + \frac{2}{3}h d\boldsymbol{\sigma}_{n+1}^p$
Re-Evaluate	$d\boldsymbol{\sigma}_{n+1} = \mathbf{M}(\boldsymbol{\sigma}_{n+1}, \boldsymbol{\epsilon}_{n+1}) d\boldsymbol{\epsilon}_{n+1}$

where the differential strain rates $d\boldsymbol{\epsilon}$ are computed via finite differences according to §4.5.

5.1.3. PECE Solver for Second-Order ODEs

Let \mathbf{x} be a vector of dependent variables obeying a differential equation of evolution $d^2\mathbf{x}(t)/dt^2 = \ddot{\mathbf{x}} = \mathbf{f}(t, \mathbf{x}, \dot{\mathbf{x}})$ subject to initial conditions $\mathbf{x}_0 = \mathbf{x}(t_0)$ and $\dot{\mathbf{x}}_0 = \dot{\mathbf{x}}(t_0)$. One may think of \mathbf{x} as being displacements and their rates $\mathbf{v} = \dot{\mathbf{x}}$ as being velocities with $\mathbf{a} = \dot{\mathbf{v}} = \ddot{\mathbf{x}}$ representing accelerations.

The two-step method put forward here incrementally solves such an ODE, returning solutions associated with the next moment in time t_{n+1} , i.e., it acquires \mathbf{x}_{n+1} & $\dot{\mathbf{x}}_{n+1}$ given knowledge of the previous \mathbf{x}_{n-1} & $\dot{\mathbf{x}}_{n-1}$ and current \mathbf{x}_n & $\dot{\mathbf{x}}_n$ solutions plus their accelerations $\ddot{\mathbf{x}}_{n-1}$ and $\ddot{\mathbf{x}}_n$ with the corrector also depending upon $\ddot{\mathbf{x}}_{n+1}$, i.e., the corrector is an implicit method.

5.1.3.1. Start-Up Algorithm

Again, multi-step methods are not self starting, so a one-step method is needed to take the first step of integration, specifically

$$\text{Predict} \quad \mathbf{x}_1^p = \mathbf{x}_0 + h\dot{\mathbf{x}}_0 + \frac{1}{2}h^2\ddot{\mathbf{x}}_0 + \mathcal{O}(h^3) \quad (5.5a)$$

$$\dot{\mathbf{x}}_1^p = \dot{\mathbf{x}}_0 + h\ddot{\mathbf{x}}_0 + \mathcal{O}(h^2) \quad (5.5b)$$

$$\text{Evaluate} \quad \ddot{\mathbf{x}}_1^p = \mathbf{f}(t_1, \mathbf{x}_1^p, \dot{\mathbf{x}}_1^p) \quad (5.5c)$$

$$\text{Correct} \quad \mathbf{x}_1 = \mathbf{x}_0 + \frac{1}{2}h(\dot{\mathbf{x}}_1^p + \dot{\mathbf{x}}_0) - \frac{1}{12}h^2(\ddot{\mathbf{x}}_1^p - \ddot{\mathbf{x}}_0) + \mathcal{O}(h^4) \quad (5.5d)$$

$$\dot{\mathbf{x}}_1 = \dot{\mathbf{x}}_0 + \frac{1}{2}h(\ddot{\mathbf{x}}_1^p + \ddot{\mathbf{x}}_0) + \mathcal{O}(h^3) \quad (5.5e)$$

$$\text{Re-Evaluate} \quad \ddot{\mathbf{x}}_1 = \mathbf{f}(t_1, \mathbf{x}_1, \dot{\mathbf{x}}_1) \quad (5.5f)$$

wherein $\ddot{\mathbf{x}}_0 = \mathbf{f}(t_0, \mathbf{x}_0, \dot{\mathbf{x}}_0)$ and $t_1 = t_0 + h$. The correct/re-evaluate steps can be iterated over until a convergence criterion is satisfied, if need be.

5.1.3.2. Two-Step ODE Solver

The two-step method of Freed [93] for solving 2nd order ODEs is

$$\begin{aligned} \text{Predict} \quad \mathbf{x}_{n+1}^p &= \frac{1}{3}(4\mathbf{x}_n - \mathbf{x}_{n-1}) + \frac{1}{6}h(3\dot{\mathbf{x}}_n + \dot{\mathbf{x}}_{n-1}) \\ &\quad + \frac{1}{36}h^2(31\ddot{\mathbf{x}}_n - \ddot{\mathbf{x}}_{n-1}) + \mathcal{O}(h^4) \end{aligned} \quad (5.6a)$$

$$\dot{\mathbf{x}}_{n+1}^p = \frac{1}{3}(4\dot{\mathbf{x}}_n - \dot{\mathbf{x}}_{n-1}) + \frac{2}{3}h(2\ddot{\mathbf{x}}_n - \ddot{\mathbf{x}}_{n-1}) + \mathcal{O}(h^3) \quad (5.6b)$$

$$\text{Evaluate} \quad \ddot{\mathbf{x}}_{n+1}^p = \mathbf{f}(t_{n+1}, \mathbf{x}_{n+1}^p, \dot{\mathbf{x}}_{n+1}^p) \quad (5.6c)$$

$$\begin{aligned} \text{Correct} \quad \mathbf{x}_{n+1} &= \frac{1}{3}(4\mathbf{x}_n - \mathbf{x}_{n-1}) + \frac{1}{24}h(\dot{\mathbf{x}}_{n+1}^p + 14\dot{\mathbf{x}}_n + \dot{\mathbf{x}}_{n-1}) \\ &\quad + \frac{1}{72}h^2(10\ddot{\mathbf{x}}_{n+1}^p + 51\ddot{\mathbf{x}}_n - \ddot{\mathbf{x}}_{n-1}) + \mathcal{O}(h^4) \end{aligned} \quad (5.6d)$$

$$\dot{\mathbf{x}}_{n+1} = \frac{1}{3}(4\dot{\mathbf{x}}_n - \dot{\mathbf{x}}_{n-1}) + \frac{2}{3}h\ddot{\mathbf{x}}_{n+1}^p + \mathcal{O}(h^3) \quad (5.6e)$$

$$\text{Re-Evaluate} \quad \ddot{\mathbf{x}}_{n+1} = \mathbf{f}(t_{n+1}, \mathbf{x}_{n+1}, \dot{\mathbf{x}}_{n+1}) \quad (5.6f)$$

where $t_{n+1} = t_n + h$. An implementation of this integrator is described in Appendix H.2.

The above PECE solver for velocity $\dot{\mathbf{x}}$ is the same method presented in Eq. (5.2), so this predictor/corrector pair is consistent. Likewise, in both the predictor and corrector for displacement \mathbf{x} , contributions from the solution \mathbf{x} have a weight of 1, contributions from the velocities $\dot{\mathbf{x}}$ have a weight of $\frac{2}{3}h$, and contributions from the accelerations $\ddot{\mathbf{x}}$ have a weight of $\frac{5}{6}h^2$; hence, this predictor/corrector pair is consistent, too. In other words, these predictor/corrector pairs produce the same results when integrating a constant acceleration field.

5.1.4. A Relevant Example

The finite element problem that we consider here requires solutions for

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{K}\mathbf{u} = \mathbf{f}(t)$$

where \mathbf{u} is a generalized displacement vector, $\ddot{\mathbf{u}}$ is its acceleration, \mathbf{M} and \mathbf{K} are mass and stiffness matrices, and $\mathbf{f}(t)$ is a forcing function evaluated at current time t . For this system of ODEs, the first step to be taken follows algorithm (5.5) and is implemented as

$$\begin{aligned} \text{Predict} \quad \mathbf{u}_1^p &= \mathbf{u}_0 + h\dot{\mathbf{u}}_0 + \frac{1}{2}h^2\ddot{\mathbf{u}}_0 \\ \dot{\mathbf{u}}_1^p &= \dot{\mathbf{u}}_0 + h\ddot{\mathbf{u}}_0 \\ \text{Evaluate} \quad \ddot{\mathbf{u}}_1^p &= \mathbf{M}^{-1}(\mathbf{f}(t_1) - \mathbf{K}\mathbf{u}_1^p) \\ \text{Correct} \quad \mathbf{u}_1 &= \mathbf{u}_0 + \frac{1}{2}h(\dot{\mathbf{u}}_1^p + \dot{\mathbf{u}}_0) - \frac{1}{12}h^2(\ddot{\mathbf{u}}_1^p - \ddot{\mathbf{u}}_0) \\ \dot{\mathbf{u}}_1 &= \dot{\mathbf{u}}_0 + \frac{1}{2}h(\ddot{\mathbf{u}}_1^p + \ddot{\mathbf{u}}_0) \\ \text{Re-Evaluate} \quad \ddot{\mathbf{u}}_1 &= \mathbf{M}^{-1}(\mathbf{f}(t_1) - \mathbf{K}\mathbf{u}_1) \end{aligned}$$

where the CE steps of the PECE sequence can be iterated on to a user-specified tolerance, which increases the methods stability as the corrector is implicit. Continued solution steps

are then governed by algorithm (5.6), which takes on the form of

$$\begin{aligned}
\text{Predict} \quad & \mathbf{u}_{n+1}^p = \frac{1}{3}(4\mathbf{u}_n - \mathbf{u}_{n-1}) + \frac{1}{6}h(3\dot{\mathbf{u}}_n + \dot{\mathbf{u}}_{n-1}) + \frac{1}{36}h^2(31\ddot{\mathbf{u}}_n - \ddot{\mathbf{u}}_{n-1}) \\
& \dot{\mathbf{u}}_{n+1}^p = \frac{1}{3}(4\dot{\mathbf{u}}_n - \dot{\mathbf{u}}_{n-1}) + \frac{2}{3}h(2\ddot{\mathbf{u}}_n - \ddot{\mathbf{u}}_{n-1}) \\
\text{Evaluate} \quad & \ddot{\mathbf{u}}_{n+1}^p = \mathbf{M}^{-1}(\mathbf{f}(t_{n+1}) - \mathbf{K}\mathbf{u}_{n+1}^p) \\
\text{Correct} \quad & \mathbf{u}_{n+1} = \frac{1}{3}(4\mathbf{u}_n - \mathbf{u}_{n-1}) + \frac{1}{24}h(\dot{\mathbf{u}}_{n+1}^p + 14\dot{\mathbf{u}}_n + \dot{\mathbf{u}}_{n-1}) \\
& \quad + \frac{1}{72}h^2(10\ddot{\mathbf{u}}_{n+1}^p + 51\ddot{\mathbf{u}}_n - \ddot{\mathbf{u}}_{n-1}) \\
& \dot{\mathbf{u}}_{n+1} = \frac{1}{3}(4\dot{\mathbf{u}}_n - \dot{\mathbf{u}}_{n-1}) + \frac{2}{3}h\ddot{\mathbf{u}}_{n+1}^p \\
\text{Re-Evaluate} \quad & \ddot{\mathbf{u}}_{n+1} = \mathbf{M}^{-1}(\mathbf{f}(t_{n+1}) - \mathbf{K}\mathbf{u}_{n+1})
\end{aligned}$$

where, again, the CE steps of the PECE sequence can be iterated on to a user-specified tolerance. In this problem, velocities $\dot{\mathbf{u}}$ are not needed for the evaluation steps, but they are required by the prediction and correction steps of integration.

We observe that the mass matrix must not be ill conditioned in order for this algorithm to work as intended. Since the mass matrix does not change with time, it only needs to be evaluated and inverted once. This is an advantage over using the popular Newmark [96] integrator where matrix inversion is required at every step along a solution path.

5.2. Quadrature Rules for Spatial Integration

Four, Gauss, quadrature rules are given here for 1D rods, 2D triangles, 2D pentagons and 3D tetrahedra, which are used in our modeling of alveoli. The formulæ provided can integrate 1st, 3rd and 5th order polynomials exactly for their respective geometries. Integrating 1st order polynomials takes place at their centroids. All integrations occur in their natural co-ordinate systems.

5.2.1. Gauss Integration of a Rod

Quadrature rules that integrate a 1D chord in its natural co-ordinate system, which spans $-1 \leq \xi \leq 1$, are presented in Table 5.1. These formulæ are well known and can be found in any finite element textbook. Here the integral of some function $f(\xi)$ is approximated via the quadrature rule

$$I = \int_{-1}^1 f(\xi) d\xi = \sum_{i=1}^n w_i f(\xi_i) + E \quad \text{where} \quad \int_{-1}^1 d\xi = \sum_{i=1}^n w_i = 2 \quad (5.9)$$

wherein ξ_i and w_i are the nodes and weights of integration, of which there are n pairs, with E denoting the error of approximation. The quadrature rules for Gauss integration are typically selected to integrate elements in a finite element model, because they have the smallest errors of approximation.

nodes	ξ co-ordinate	weight
Exact for Polynomials of Degree 1		
1	0.000000000000000	2.000000000000000
Exact for Polynomials of Degree 3		
1	-0.577350269189626	1.000000000000000
2	0.577350269189626	1.000000000000000
Exact for Polynomials of Degree 5		
1	-0.774596669241483	0.5555555555555556
2	0.000000000000000	0.8888888888888889
3	0.774596669241483	0.5555555555555556

Table 5.1: Gauss quadrature weights and nodes for integrating over a line in its natural co-ordinate system ξ . These weights sum to 2, which is the span of its natural co-ordinate. We note that $1/\sqrt{3} \approx 0.577350269189626$ and that $\sqrt{3}/5 \approx 0.774596669241483$.

5.2.2. Multi-Dimensional Integration

When integrating a function f over, e.g., a square, one often introduces tensor products of the 1D formulæ (5.9) listed in Table 5.1; specifically, one might construct integration quadratures that look like

$$I = \int_{-1}^1 \int_{-1}^1 f(\xi, \eta) d\xi d\eta = \int_{-1}^1 \sum_{i=1}^n w_i f(\xi_i, \eta) d\eta + E = \sum_{i=1}^n \sum_{j=1}^n w_i w_j f(\xi_i, \eta_j) + E$$

which is the integration scheme presented in many textbooks on finite elements. However, these formulæ are not optimal, because they require many more function evaluations than are necessary in order to secure a quadrature at a specified accuracy. It is much more efficient to adopt non-tensor product quadratures where, when integrating over a square, one has

$$I = \int_{-1}^1 \int_{-1}^1 f(\xi, \eta) d\xi d\eta = \sum_{i=1}^n w_i f(\xi_i, \eta_i) + E \quad \text{where} \quad \int_{-1}^1 \int_{-1}^1 d\xi d\eta = \sum_{i=1}^n w_i = 4$$

with co-ordinates ξ_i and η_i placing the i^{th} node of integration inside a square of area 4 whose corresponding weight of integration is w_i , with their being n pairs of nodes and weights.

It is this latter formula that we employ for our multi-dimensional integrations.

5.2.3. Gauss Integration of a Triangle

The triangle considered has natural co-ordinates (ξ, η) that span $0 \leq \xi \leq 1 - \eta$ and $0 \leq \eta \leq 1$ so that the integral of interest becomes

$$I = \int_0^1 \int_{\xi=0}^{1-\eta} f(\xi, \eta) d\xi d\eta = \sum_{i=1}^n w_i f(\xi_i, \eta_i) + E \quad \text{where} \quad \int_0^1 \int_{\xi=0}^{1-\eta} d\xi d\eta = \sum_{i=1}^n w_i = \frac{1}{2} \quad (5.10)$$

with co-ordinates ξ_i and η_i placing the i^{th} node of integration inside the triangle whose corresponding weight of integration is w_i , with their being n pairs of nodes and weights. The area of this triangle is $1/2$, the sum of its weights. Table 5.2 provides a selection of quadratures for such triangles. This table can be found in some finite element textbooks.

nodes	ξ co-ordinate	η co-ordinate	weight
Exact for Polynomials of Degree 1			
1	0.3333333333333333	0.3333333333333333	0.5000000000000000
Exact for Polynomials of Degree 3			
1	0.3333333333333333	0.3333333333333333	-0.2812500000000000
2	0.2000000000000000	0.6000000000000000	0.2604166666666667
3	0.2000000000000000	0.2000000000000000	0.2604166666666667
4	0.6000000000000000	0.2000000000000000	0.2604166666666667
Exact for Polynomials of Degree 5			
1	0.3333333333333333	0.3333333333333333	0.1125000000000000
2	0.101286507323456	0.797426985353087	0.062969590272413
3	0.101286507323456	0.101286507323456	0.062969590272413
4	0.797426985353087	0.101286507323456	0.062969590272413
5	0.470142064105115	0.059715871789770	0.066197076394253
6	0.470142064105115	0.470142064105115	0.066197076394253
7	0.059715871789770	0.470142064105115	0.066197076394253

Table 5.2: Gauss quadrature weights and nodes for integrating over a triangle in its natural co-ordinate system (ξ, η) , where $0 \leq \xi \leq 1 - \eta$ and $0 \leq \eta \leq 1$. These weights sum to $1/2$, which is the area of a triangle when evaluated in its natural co-ordinate system.

5.2.4. Gauss Integration of a Pentagon

Gauss quadrature rules for a regular pentagon described in its natural coordinate system, i.e., oriented according to Fig. 2.2, are presented in Table 5.3, which describe integrations of the type

$$\iint_{\triangle} f(\xi, \eta) d\xi d\eta = \sum_{i=1}^n w_i f(\xi_i, \eta_i) + E$$

with $\iint_{\triangle} d\xi d\eta = \sum_{i=1}^n w_i = A^p = 5 \sin \omega \cos \omega = 2.3776412907378837$ (5.11)

where co-ordinates ξ_i and η_i place the i^{th} node inside the pentagon whose corresponding weight of integration is w_i , with their being n pairs of nodes and weights, and where A^p is the area of this pentagon with $2\omega = 108^\circ$ being an inside angle of this regular pentagon.

The quadratures presented in Table 5.3 were supplied to the authors by Prof. N. Sukumar from the University of California at Davis, which he derived for us at our request using a methodology that he published in Ref. [97]. In that document, the authors derived formulæ for determining the nodes and weights for a class of generalized, Gaussian, quadrature rules, which they then applied to pentagons, hexagons, heptagons and octagons, of which they only published their nodes and weights of quadrature for the hexagon, as it tiles two space. The node for the 1st order method is located at the centroid. Nodes for the 3rd and 5th order methods of Table 5.3 are displayed in Fig. 5.1.

node	ξ co-ordinate	η co-ordinate	weight
Exact for Polynomials of Degree 1			
1	0.0000000000000000	0.0000000000000000	2.3776412907378837
Exact for Polynomials of Degree 3			
1	-0.0349156305831802	0.6469731019095136	0.5449124407446143
2	-0.5951653065516678	-0.0321196846022659	0.6439082046243272
3	0.0349156305831798	-0.6469731019095134	0.5449124407446146
4	0.5951653065516677	0.0321196846022661	0.6439082046243275
Exact for Polynomials of Degree 5			
1	-0.0000000000000000	-0.0000000000000002	0.6257871064166934
2	-0.1351253857178451	0.7099621260052327	0.3016384608809768
3	-0.6970858746672087	0.1907259121533272	0.3169910433902452
4	-0.4651171392611024	-0.5531465782166917	0.3155445150066620
5	0.2842948078559476	-0.6644407817506509	0.2958801959111726
6	0.7117958231685716	-0.1251071394727008	0.2575426306970870
7	0.5337947578638855	0.4872045224587945	0.2642573384350463

Table 5.3: Gauss quadrature weights and nodes (a.k.a., cubature rules) for integrating over a regular pentagon in its natural coordinate system (ξ, η) . These weights sum to the area of a pentagon inscribing an unit circle, the formula of which is given in Eqn. (2.6).

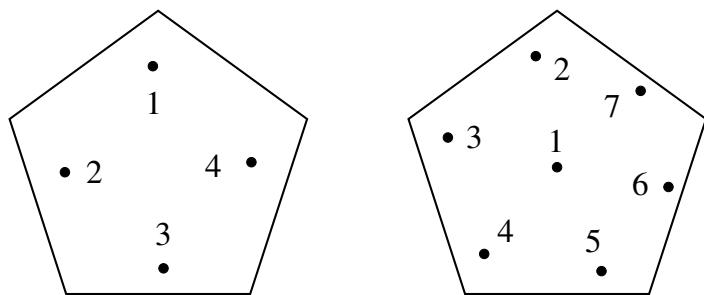


Figure 5.1: Locations of generalized, Gaussian, quadrature nodes for the 3rd (left) and 5th (right) degree integration methods presented in Table 5.3. Vertex 1 is located at the top of the pentagon, cf. Fig. 2.2, while the coordinate origin is located at its centroid (node 1 in the right figure).

The Gaussian quadrature rules of Mousavi, Xiao & Sukumar [97] presented in Table 5.3 are compatible with the shape functions of Wachspress [43, 44] and Dasgupta [47] presented in §3.3.1.

5.2.5. Gauss Integration of a Tetrahedron

Integrating over the volume of a tetrahedron, when expressed in its natural co-ordinates (ξ, η, ζ) that span $0 \leq \xi \leq 1 - \eta - \zeta$, $0 \leq \eta \leq 1 - \zeta$ and $0 \leq \zeta \leq 1$ so that the integral of interest becomes

$$I = \int_0^1 \int_{\eta=0}^{1-\zeta} \int_{\xi=0}^{1-\eta-\zeta} f(\xi, \eta, \zeta) d\xi d\eta d\zeta = \sum_{i=1}^n w_i f(\xi_i, \eta_i, \zeta_i) + E$$

where $\int_0^1 \int_{\eta=0}^{1-\zeta} \int_{\xi=0}^{1-\eta-\zeta} d\xi d\eta d\zeta = \sum_{i=1}^n w_i = \frac{1}{6}$ (5.12)

with co-ordinates ξ_i , η_i and ζ_i placing the i^{th} node of integration inside the tetrahedron whose corresponding weight of integration is w_i , with there being n pairs of nodes and weights. The volume of this tetrahedron is $1/6$. Table 5.4 provides a selection of quadratures for tetrahedra when mapped into their natural co-ordinate system. This table can be found in some finite element textbooks.

node	ξ co-ordinate	η co-ordinate	ζ co-ordinate	weight
Exact for Polynomials of Degree 1				
1	0.250000000000000	0.250000000000000	0.250000000000000	0.166666666666667
Exact for Polynomials of Degree 3				
1	0.250000000000000	0.250000000000000	0.250000000000000	-0.133333333333333
2	0.500000000000000	0.166666666666667	0.166666666666667	0.075000000000000
3	0.166666666666667	0.500000000000000	0.166666666666667	0.075000000000000
4	0.166666666666667	0.166666666666667	0.500000000000000	0.075000000000000
5	0.166666666666667	0.166666666666667	0.166666666666667	0.075000000000000
Exact for Polynomials of Degree 5				
1	0.250000000000000	0.250000000000000	0.250000000000000	0.030283678097089
2	0.000000000000000	0.333333333333333	0.333333333333333	0.006026785714286
3	0.333333333333333	0.000000000000000	0.333333333333333	0.006026785714286
4	0.333333333333333	0.333333333333333	0.000000000000000	0.006026785714286
5	0.333333333333333	0.333333333333333	0.333333333333333	0.006026785714286
6	0.727272727272727	0.090909090909091	0.090909090909091	0.011645249086029
7	0.090909090909091	0.727272727272727	0.090909090909091	0.011645249086029
8	0.090909090909091	0.090909090909091	0.727272727272727	0.011645249086029
9	0.090909090909091	0.090909090909091	0.090909090909091	0.011645249086029
10	0.066550153573664	0.433449846426336	0.433449846426336	0.010949141561386
11	0.433449846426336	0.066550153573664	0.433449846426336	0.010949141561386
12	0.433449846426336	0.433449846426336	0.066550153573664	0.010949141561386
13	0.433449846426336	0.066550153573664	0.066550153573664	0.010949141561386
14	0.066550153573664	0.433449846426336	0.066550153573664	0.010949141561386
15	0.066550153573664	0.066550153573664	0.433449846426336	0.010949141561386

Table 5.4: Gauss quadrature weights and nodes for integrating over a tetrahedron in its natural co-ordinate system (ξ, η, ζ) , where $0 \leq \xi \leq 1 - \eta - \zeta$, $0 \leq \eta \leq 1 - \zeta$ and $0 \leq \zeta \leq 1$. These weights sum to $1/6$, which is the volume of a tetrahedron measured in its natural co-ordinate system.

Part 6

Variational Formulation

The problem we have set up to solve takes on the general form of a second-order, hyperbolic, ordinary, differential equation; specifically,

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{K}\mathbf{u} = \mathbf{f}(t) \quad (6.1)$$

where \mathbf{M} is a mass matrix, \mathbf{K} is a stiffness matrix, \mathbf{f} is a forcing function dependent upon time t , and \mathbf{u} is a displacement vector with $\ddot{\mathbf{u}}$ denoting acceleration. At present, a possible contribution arising from dissipation is not included, e.g., a $\mathbf{C}\dot{\mathbf{u}}$ term accounting for visco-elastic effects. The numerical solution strategy employed to solve this ODE is discussed in §5.1.4, which requires \mathbf{M} to be an invertible matrix.

A dodecahedron used to model an alveolar sac is our problem of interest. The shape of an irregular dodecahedron is described by a set of 20 vertices, each experiencing a displacement

$$\mathbf{u}_i = \{u_{xi}, u_{yi}, u_{zi}\}^\top := \{x_i - x_{0i}, y_i - y_{0i}, z_i - z_{0i}\}^\top, \quad i = 1, 2, \dots, 20 \quad (6.2)$$

that contains co-ordinate differences at a dodecahedral vertex evaluated in the physical co-ordinate frame of this dodecahedron ($\vec{\mathbf{E}}_1, \vec{\mathbf{E}}_2, \vec{\mathbf{E}}_3$), as established in §2.1, with each vertex i having reference co-ordinates denoted as $\{x_{0i}, y_{0i}, z_{0i}\}^\top$ and current co-ordinates denoted as $\{x_i, y_i, z_i\}^\top$. The 20 vertices of a dodecahedron uniquely establish its 30 alveolar chords, its 12 alveolar septa, and the alveolar sac that these chords and septa envelop, cf. §2.6.

When assembled, vectors \mathbf{f} , \mathbf{u} and $\ddot{\mathbf{u}}$ have lengths of 60 for the alveolar chord and septa models, and a length of 63 for the alveolar sac model, while matrices \mathbf{M} and \mathbf{K} have dimensions of 60×60 for the alveolar chord and septa models, and dimensions of 63×63 for the alveolar sac model. The model for alveolar volume has an extra node located at the centroid of the dodecahedron, which is a node in common betwixt the 60 tetrahedra needed to fill the volume of a dodecahedron in our modeling of an alveolus.

As a modeling simplification, the alveolar chords, the alveolar septa, and the alveolar sac are each modeled separately. It is the nodal forces resulting from these three, separate, finite-element models that then are summed. These are obtained by interpolating the stresses integrated at their Guass points out to their nodes, which belong to the set dodecahedral vertices. These three sources for vertex force can be added, from which an uniform (homogenized) state of stress can then be calculated for return.

Consequently, we are constructing three, individual, finite-element models governed by the following systems of hyperbolic differential equations

$$\mathbf{M}_{1D}\ddot{\mathbf{u}} + \mathbf{K}_{1D}\mathbf{u} = \mathbf{f}_{1D}(t) \quad (6.3a)$$

$$\mathbf{M}_{2D}\ddot{\mathbf{u}} + \mathbf{K}_{2D}\mathbf{u} = \mathbf{f}_{2D}(t) \quad (6.3b)$$

$$\mathbf{M}_{3D}\ddot{\mathbf{u}} + \mathbf{K}_{3D}\mathbf{u} = \mathbf{f}_{3D}(t) \quad (6.3c)$$

where subscript ' $1D$ ' designates alveolar chords, subscript ' $2D$ ' designates alveolar septa, and subscript ' $3D$ ' designates an alveolar sac. It is thought to be necessary to split the overall problem into these three subproblems due to the vast differences in their compliance moduli.

6.1. Mass Matrix

A consistent mass matrix [98] for an element, established in its natural co-ordinate system, is defined as

$$\mathbf{M}_C = \int_V \rho \mathbf{N}^T \mathbf{N} dV \quad (6.4)$$

wherein \mathbf{N} is the shape function matrix for an element whose mass density is ρ . This mass matrix is said to be consistent in that it is calculated with the same shape functions that are used to create the stiffness matrix. Consistent mass matrices are symmetric and, sometimes, they are singular, too, which is not a desirable feature for our chosen numerical approach.

To construct a non-singular mass matrix, we introduce a lumped mass matrix. Specifically, the sum of all row elements from each row of a consistent mass matrix establishes the diagonal elements of a lumped mass matrix [99] in that

$$\mathbf{M}_L = \sum_{i=1}^n M_{Li} \quad \text{where} \quad M_{Li} = \sum_{j=1}^n \int_V \rho N_i N_j dV \quad (6.5)$$

wherein $\sum_{j=1}^n N_j = 1$ with i being a Gauss point out of the n Gauss points in an element.

A lumped-consistent (or weighted) mass matrix \mathbf{M}_W can then be defined as follows

$$\mathbf{M}_W = (1 - \mu) \mathbf{M}_C + \mu \mathbf{M}_L \quad (6.6)$$

wherein μ is a free scalar parameter for weighting the consistent and lumped mass matrices. The reason for mixing \mathbf{M}_C and \mathbf{M}_L is that the weighted matrix \mathbf{M}_W will not be singular. Herein μ is taken to be a half, i.e., an averaged mass matrix is adopted, which has a nice property of minimizing low frequency dispersion. Specifically,

$$\mathbf{M}_A = \frac{1}{2} (\mathbf{M}_C + \mathbf{M}_L) \quad (6.7)$$

is how we shall construct our mass matrices. The averaged mass matrix \mathbf{M}_A is invertible, which is a requirement of the selected numerical solution strategy presented in §5.1.4.

6.1.1. Mass Matrices for a Chord

A two-noded alveolar chord has shape functions N_i that, when evaluated in its natural co-ordinate system wherein $-1 \leq \xi \leq 1$, aggregate into a matrix of shape functions

$$\mathbf{N} = [N_1 \ N_2] = \left[\frac{1}{2}(1 - \xi) \ \frac{1}{2}(1 + \xi) \right] \quad \text{so that} \quad N_{1,\xi} = -\frac{1}{2} \quad \text{and} \quad N_{2,\xi} = \frac{1}{2} \quad (6.8)$$

where ξ is the abscissa associated with a specific Gauss integration rule, cf. Table 5.1.

The Jacobian matrix \mathbf{J} for a one-dimensional chord, which is also its Jacobian determinant $|\mathbf{J}|$, is used to transform the integrals in Eqns. (6.4 & 6.5) from their global co-ordinate system into their natural co-ordinate system. It has a value of

$$\mathbf{J} \equiv |\mathbf{J}| = \sum_{i=1}^2 N_{i,\xi}(\xi) x_i = -\frac{1}{2} \cdot -\frac{1}{2}L + \frac{1}{2} \cdot \frac{1}{2}L = \frac{1}{2}L \quad (6.9)$$

given nodal co-ordinates of $x_1 = -\frac{1}{2}L$ and $x_2 = \frac{1}{2}L$, where L is the length of our alveolar chord. The Jacobian matrix and the Jacobian determinant are equal in this case because the space is one dimensional.

The consistent mass matrix for a 1D alveolar chord modeled as a two-noded rod, when evaluated in its natural co-ordinate system, becomes

$$\begin{aligned}\mathbf{M}_{1C} &= \int_0^L \rho \mathbf{N}^T \mathbf{N} A dx = \int_{-1}^1 \rho \mathbf{N}^T \mathbf{N} A |\mathbf{J}| d\xi \\ &= \sum_{i=1}^n \rho N_i^T N_i A |\mathbf{J}| w_i = \sum_{i=1}^n \frac{\rho AL w_i}{8} \begin{bmatrix} 1 - 2\xi_i + \xi_i^2 & 1 - \xi_i^2 \\ 1 - \xi_i^2 & 1 + 2\xi_i + \xi_i^2 \end{bmatrix}\end{aligned}\quad (6.10)$$

with N_i and w_i being the shape functions and weights of quadrature for the selected Gauss integration rule evaluated at Gauss point i , while A is the cross-sectional area of our alveolar chord. Table 5.1 presents values for the abscissæ ξ_i and weights w_i of integration for schemes where there are $n = 1, 2$ or 3 nodes of integration along an alveolar chord.

The lumped mass matrix for a 1D alveolar chord in its natural co-ordinate system is

$$\begin{aligned}\mathbf{M}_{1L} &= \sum_{i,j=1}^n \int_0^L \rho N_i N_j A dx = \sum_{i=1}^n \int_{-1}^1 \rho N_i A |\mathbf{J}| d\xi \\ &= \sum_{i=1}^n \rho N_i A |\mathbf{J}| w_i = \sum_{i=1}^n \frac{\rho AL w_i}{4} \begin{bmatrix} 1 - \xi_i & 0 \\ 0 & 1 + \xi_i \end{bmatrix}\end{aligned}\quad (6.11)$$

because $\sum_{j=1}^n N_j = 1$. It is readily apparent that the mass matrix in Eqn. (6.10) at a Gauss point is singular, whereas the mass matrix in Eqn. (6.11) has a reciprocal, except at $\xi = \pm 1$.

Chordal mass matrices associated with the Gauss quadratures listed in Table 5.1 become: The consistent mass matrices for a chord are

$$\mathbf{M}_{1C} = \frac{\rho AL}{4} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \quad \mathbf{M}_{1C} = \frac{\rho AL}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \quad \mathbf{M}_{1C} = \frac{\rho AL}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \quad (6.12a)$$

The lumped mass matrices for a chord are

$$\mathbf{M}_{1L} = \frac{\rho AL}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \mathbf{M}_{1L} = \frac{\rho AL}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \mathbf{M}_{1L} = \frac{\rho AL}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (6.12b)$$

When averaged these mass matrices become

$$\mathbf{M}_{1A} = \frac{\rho AL}{8} \begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix} \quad \mathbf{M}_{1A} = \frac{\rho AL}{12} \begin{bmatrix} 5 & 1 \\ 1 & 5 \end{bmatrix} \quad \mathbf{M}_{1A} = \frac{\rho AL}{12} \begin{bmatrix} 5 & 1 \\ 1 & 5 \end{bmatrix} \quad (6.12c)$$

which are the mass matrices that we employ. This collection of mass matrices pertain to one Gauss point (left set of mass matrices), two Gauss points (center set of mass matrices), and three Gauss points (right set of mass matrices). For this element, there is no difference between the mass matrices for two and three Gauss points of integration. In the derivation of these matrices, it is assumed that the cross-sectional area and mass density are both uniform along the length of a septal chord. Furthermore, because septal chord volume V is considered to be preserved, i.e., $V = V_0$ where $V_0 = A_0 L_0$ and $V = AL$, it follows that these mass matrices are constant; hence, their inverses need only be determined once.

6.1.1.1. Assemble Mass Matrices for the Septal Chords

6.1.2. Mass Matrices for a Pentagon

For an alveolar septa represented as an irregular pentagon, its matrix of shape functions \mathbf{N} takes on the form of

$$\mathbf{N} = \begin{bmatrix} N_1 & 0 & N_2 & 0 & N_3 & 0 & N_4 & 0 & N_5 & 0 \\ 0 & N_1 & 0 & N_2 & 0 & N_3 & 0 & N_4 & 0 & N_5 \end{bmatrix} \quad (6.13)$$

where N_i , $i = 1, \dots, 5$, are the five shape functions that correspond with the five vertices of a pentagon, as established in Eqn. (3.6).

A consistent mass matrix \mathbf{M}_{2C} is constructed by substituting the above matrix of shape functions into the following expression

$$\mathbf{M}_{2C} = \iint_{\triangle} \rho \mathbf{N}^T \mathbf{N} |\mathbf{J}| h d\xi d\eta \quad (6.14)$$

with h denoting membrane thickness, and where $|\mathbf{J}|$ denotes the determinant of a 2×2 Jacobian matrix for a pentagon. In quadrilateral derivations, a Jacobian of two-dimensional transformations that connect the physical x, y to natural ξ, η co-ordinate systems is needed. The components of this Jacobian matrix are calculated using derivatives of shape functions taken with respect to the local co-ordinates at the i^{th} vertex via

$$\mathbf{J} = \begin{bmatrix} \partial x / \partial \xi & \partial y / \partial \xi \\ \partial x / \partial \eta & \partial y / \partial \eta \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^5 N_{i,\xi}(\xi, \eta) x_i & \sum_{i=1}^5 N_{i,\xi}(\xi, \eta) y_i \\ \sum_{i=1}^5 N_{i,\eta}(\xi, \eta) x_i & \sum_{i=1}^5 N_{i,\eta}(\xi, \eta) y_i \end{bmatrix} \quad (6.15)$$

where the shape function gradients $N_{i,\xi}$ and $N_{i,\eta}$ have been established in Eqn. (3.10), with

$$\mathbf{J}^{-1} = \frac{1}{|\mathbf{J}|} \begin{bmatrix} \partial y / \partial \eta & -\partial y / \partial \xi \\ -\partial x / \partial \eta & \partial x / \partial \xi \end{bmatrix} \quad \text{wherein} \quad |\mathbf{J}| = \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} - \frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \xi} \quad (6.16)$$

providing its inverse and Jacobian determinant. A numerical integration of Eqn. (6.14) results in

$$\mathbf{M}_{2C} = \sum_{i=1}^n \rho \mathbf{N}^T(\xi_i, \eta_i) \mathbf{N}(\xi_i, \eta_i) |\mathbf{J}| h w_i \quad (6.17)$$

where n stands for the number of Gauss points, and where w_i and w_j denote the weights of quadrature in an element's natural co-ordinate system, which can be found in Table 5.3.

A lumped mass matrix for a pentagon gets its diagonal elements as follows

$$M_{2Li} = \sum_{j=1}^n \iint_{\triangle} \rho N_i N_j |\mathbf{J}| h d\xi d\eta = \sum_{i=1}^n \rho N(\xi_i, \eta_i) |\mathbf{J}| h w_i \quad (6.18)$$

because $\sum_{j=1}^n N_j = 1$.

For instance, the averaged lumped-consistent mass matrix for a pentagon with 1 Gauss point of integration located at its centroid is constructed by averaging its consistent and lumped mass matrices resulting in

$$\mathbf{M}_{2A} = \frac{\rho h A}{100} \begin{bmatrix} 6 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 6 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 6 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 6 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 6 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 6 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 6 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 6 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 6 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 6 \end{bmatrix} \quad (6.19)$$

where h and A are the thickness and area of the membrane. It just so happens that, in this case, the mass matrix turns out nice. Because septal volume V is considered to be preserved, i.e., $V = V_0$ where $V_0 = h_0 A_0$ and $V = hA$, it follows that this mass matrix is constant; hence, its inverse need only be determined once.

Three mass matrices have been constructed for a pentagon based upon the three, Gauss, quadrature rules presented in Table 5.3, which integrate polynomials of orders 1, 3 and 5 exactly, respectively.

6.1.2.1. Assemble Mass Matrices for the Alveolar Septa

6.1.3. Mass Matrices for a Tetrahedron

A dodecahedron has 60 individual tetrahedra contained within it, whose centroid is a common vertex to all 60 of these tetrahedra. Hence, an analysis to find the mass matrix of a tetrahedron is used as the building block needed to assemble the mass matrix for an alveolar sac.

The matrix of shape functions \mathbf{N} for a tetrahedron has the form of

$$\mathbf{N} = \begin{bmatrix} N_1 & 0 & 0 & N_2 & 0 & 0 & N_3 & 0 & 0 & N_4 & 0 & 0 \\ 0 & N_1 & 0 & 0 & N_2 & 0 & 0 & N_3 & 0 & 0 & N_4 & 0 \\ 0 & 0 & N_1 & 0 & 0 & N_2 & 0 & 0 & N_3 & 0 & 0 & N_4 \end{bmatrix} \quad (6.20)$$

in which N_i , $i = 1, 2, 3, 4$, are the four shape functions corresponding to the four vertices of a tetrahedron that are defined as follows

$$N_1 = 1 - \xi - \eta - \zeta \quad (6.21a)$$

$$N_2 = \xi \quad (6.21b)$$

$$N_3 = \eta \quad (6.21c)$$

$$N_4 = \zeta. \quad (6.21d)$$

Numerical integration is used to obtain the mass matrix of a tetrahedron via

$$\begin{aligned}\mathbf{M}_{3C} &= \iiint_V \rho \mathbf{N}^T \mathbf{N} d\mathbf{x} dy dz = \int_0^1 \int_0^1 \int_0^1 \rho \mathbf{N}^T \mathbf{N} |\mathbf{J}| d\xi d\eta d\zeta \\ &= \sum_{i=1}^n \rho \mathbf{N}^T(\xi_i, \eta_i, \zeta_i) \mathbf{N}(\xi_i, \eta_i, \zeta_i) |\mathbf{J}| w_i\end{aligned}\quad (6.22)$$

with $|\mathbf{J}|$ being the determinant of the Jacobian matrix, and n denoting the number of Gauss points used for integration. The Jacobian is calculated from derivatives of the shape functions taken with respect to its local co-ordinates (ξ, η, ζ) that associate with their current global co-ordinates (x_i, y_i, z_i) according to

$$\begin{aligned}\mathbf{J} &= \begin{bmatrix} \partial x / \partial \xi & \partial y / \partial \xi & \partial z / \partial \xi \\ \partial x / \partial \eta & \partial y / \partial \eta & \partial z / \partial \eta \\ \partial x / \partial \zeta & \partial y / \partial \zeta & \partial z / \partial \zeta \end{bmatrix} = \begin{bmatrix} x_{,\xi} & y_{,\xi} & z_{,\xi} \\ x_{,\eta} & y_{,\eta} & z_{,\eta} \\ x_{,\zeta} & y_{,\zeta} & z_{,\zeta} \end{bmatrix} \\ &= \begin{bmatrix} \sum_{i=1}^4 N_{i,\xi}(\xi, \eta, \zeta) x_i & \sum_{i=1}^4 N_{i,\xi}(\xi, \eta, \zeta) y_i & \sum_{i=1}^4 N_{i,\xi}(\xi, \eta, \zeta) z_i \\ \sum_{i=1}^4 N_{i,\eta}(\xi, \eta, \zeta) x_i & \sum_{i=1}^4 N_{i,\eta}(\xi, \eta, \zeta) y_i & \sum_{i=1}^4 N_{i,\eta}(\xi, \eta, \zeta) z_i \\ \sum_{i=1}^4 N_{i,\zeta}(\xi, \eta, \zeta) x_i & \sum_{i=1}^4 N_{i,\zeta}(\xi, \eta, \zeta) y_i & \sum_{i=1}^4 N_{i,\zeta}(\xi, \eta, \zeta) z_i \end{bmatrix}\end{aligned}\quad (6.23)$$

with

$$\mathbf{J}^{-1} = \frac{1}{|\mathbf{J}|} \begin{bmatrix} y_{,\eta} z_{,\zeta} - z_{,\eta} y_{,\zeta} & z_{,\xi} y_{,\zeta} - y_{,\xi} z_{,\zeta} & y_{,\xi} z_{,\eta} - y_{,\eta} z_{,\xi} \\ z_{,\eta} x_{,\zeta} - x_{,\eta} z_{,\zeta} & x_{,\xi} z_{,\zeta} - z_{,\xi} x_{,\zeta} & z_{,\xi} x_{,\eta} - x_{,\xi} z_{,\eta} \\ x_{,\eta} y_{,\zeta} - y_{,\eta} x_{,\zeta} & y_{,\xi} x_{,\zeta} - x_{,\xi} y_{,\zeta} & y_{,\eta} x_{,\xi} - y_{,\xi} x_{,\eta} \end{bmatrix}\quad (6.24)$$

establishing its inverse.

For instance, the averaged lumped-consistent mass matrix for a tetrahedron with 1 Gauss point of integration located at its centroid is

$$\mathbf{M}_{3A} = \frac{\rho V}{96} \begin{bmatrix} 5 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 5 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 5 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 5 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 5 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 5 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & 5 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 5 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 5 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 5 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 5 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 5 \end{bmatrix}\quad (6.25)$$

where the volume V varies with deformation because air is compressible. The other cases are not as simple.

Three mass matrices for a tetrahedron are implemented based upon the three, Gauss, quadrature rules presented in Table 5.4. These quadratures integrate polynomials of order 1, 2 and 3, respectively.

6.1.3.1. Assemble Tetrahedral Mass Matrices to Get Mass Matrix for an Alveolar Sac

6.2. Stiffness Matrix

For a nonlinear elastic material, like a soft tissue, the stress-strain response generally becomes stiffer with increasing deformation. Consequently, the slope along their stress-strain curve changes with strain and, therefore, its instantaneous stiffness changes, too. Therefore, tangent stiffness matrices are required for our finite element simulations.

The total potential energy of a deformed body can be expressed as the difference between a variation in the potential energy of deformation δU and a variation in the potential energy of the external loading δW [100]

$$\delta R = \delta U - \delta W \quad (6.26a)$$

with

$$\delta W = \mathbf{F} d\Delta \quad (6.26b)$$

$$\delta U = \int_V \bar{\mathbf{B}}^T \mathbf{T} dV d\Delta \quad (6.26c)$$

where \mathbf{F} is a vector of external forces, \mathbf{T} are the conjugate stresses to our strains, and $\bar{\mathbf{B}}$ is a matrix relation between strain \mathbf{E} and nodal displacements Δ such that

$$\mathbf{E} = \bar{\mathbf{B}} \Delta \quad \text{with} \quad d\mathbf{E} = \bar{\mathbf{B}} d\Delta \quad (6.27)$$

with displacement fields being interpolated as

$$\bar{\mathbf{u}} = \begin{Bmatrix} u \\ v \end{Bmatrix} = \begin{Bmatrix} \sum_{i=1}^n u_i N_i \\ \sum_{i=1}^n v_i N_i \end{Bmatrix} = \mathbf{N} \Delta. \quad (6.28)$$

The total strain-displacement matrix can be defined as a sum of linear and nonlinear strain displacements as follow

$$\bar{\mathbf{B}} = \mathbf{B}_L + \mathbf{B}_N \quad (6.29)$$

where \mathbf{B}_L is obtained from linear analysis, i.e., $\mathbf{E}_L = \mathbf{B}_L \Delta$, with \mathbf{B}_N being that function of displacements \mathbf{u} which can be obtained from the nonlinear part of strain \mathbf{E}_N . It can be formed as follow

$$\mathbf{E}_N = \frac{1}{2} \mathbf{A} \boldsymbol{\theta} \quad (6.30)$$

with \mathbf{A} being a matrix of derivatives of displacement, and $\boldsymbol{\theta}$ being a vector of derivatives of displacement that can be expressed as $\boldsymbol{\theta} = \mathbf{H} \Delta$, or in rate form as $d\boldsymbol{\theta} = \mathbf{H} d\Delta$, where \mathbf{H} is the derivative of shape functions taken respect to the global co-ordinate system. Thus, the derivative of strain takes on the form of

$$d\mathbf{E} = d(\mathbf{E}_L + \mathbf{E}_N) = d\mathbf{E}_N = \frac{1}{2} (d\mathbf{A} \boldsymbol{\theta} + \mathbf{A} d\boldsymbol{\theta}) = \mathbf{A} \mathbf{H} d\Delta. \quad (6.31)$$

Rewriting Eqn. (6.29) in incremental form yields $d\bar{\mathbf{B}} = d(\mathbf{B}_L + \mathbf{B}_N) = d\mathbf{B}_N$, where the nonlinear strain displacement and its incremental form can be obtained as follow

$$\mathbf{B}_N = \mathbf{A} \mathbf{H} \quad \text{with} \quad d\mathbf{B}_N = d\mathbf{A} \mathbf{H} \quad (6.32)$$

wherein $d\mathbf{A} = \mathbf{A}' d\Delta$.

In order to satisfy the equilibrium, the first variation of the total potential energy, which is known as the residual force, should be zero [101], viz.,

$$\mathbf{R} = \int_V \bar{\mathbf{B}}^T \mathbf{T} dV - \mathbf{F} = 0 \quad (6.33)$$

whose derivative yields

$$d\mathbf{R} = \int_V d\bar{\mathbf{B}}^T \mathbf{T} dV + \int_V \bar{\mathbf{B}}^T d\mathbf{T} dV \quad (6.34)$$

where $d\mathbf{T} = \mathbf{M} d\mathbf{E} = \mathbf{M} \bar{\mathbf{B}} d\Delta$, with \mathbf{M} being the matrix of elastic tangent moduli.

The tangent stiffness matrix can be obtained by substituting the definition of $d\mathbf{T}$ into Eq. (6.34) as follow

$$\begin{aligned} d\mathbf{R} &= \int_V d\mathbf{B}_N^T \mathbf{T} dV + \int_V \bar{\mathbf{B}}^T \mathbf{M} \bar{\mathbf{B}} dV d\Delta \\ &= \int_V (\mathbf{H}^T d\mathbf{A}^T \mathbf{T}) dV + \int_V (\mathbf{B}_L + \mathbf{B}_N)^T \mathbf{M} (\mathbf{B}_L + \mathbf{B}_N) dV d\Delta \\ &= \mathbf{K}_S d\Delta + \int_V \mathbf{B}_L^T \mathbf{M} \mathbf{B}_L dV d\Delta \\ &\quad + \int_V (\mathbf{B}_L^T \mathbf{M} \mathbf{B}_N + \mathbf{B}_N^T \mathbf{M} \mathbf{B}_L + \mathbf{B}_N^T \mathbf{M} \mathbf{B}_N) dV d\Delta \\ &= (\mathbf{K}_S + \mathbf{K}_L + \mathbf{K}_N) d\Delta = \mathbf{K}_T d\Delta \end{aligned} \quad (6.35)$$

wherein \mathbf{K}_S being the stiffness matrix associated with the initial stress, \mathbf{K}_L being the conventional small displacement stiffness matrix, \mathbf{K}_N being the large displacement stiffness matrix, and \mathbf{K}_T being the total tangent-stiffness matrix.

6.2.1. Stiffness Matrix for Chord

The components of Laplace stretch \mathcal{U} have a Cholesky factorization expressed in terms of the right Cauchy-Green deformation tensor $\mathbf{C} = \mathbf{F}^T \mathbf{F} = \mathcal{U}^T \mathcal{U}$, which is a symmetric second-order tensor. A 1-D chord has an axial strain of $e = \ln(a/a_0) \equiv \ln(L/L_0)$ where L is the length of the chord, a is the 11 component of Laplace stretch that can be written in terms of the derivatives of displacement as follows

$$a = \mathcal{U}_{11} = \sqrt{C_{11}} \quad \text{with} \quad C_{11} = \left(\frac{\partial u}{\partial x} \right)^2 + 2 \frac{\partial u}{\partial x} + 1 \quad (6.36)$$

which presumes that $a_0 = 1$. The total axial strain of a chord can therefore be expressed in terms of linear and nonlinear strain increments as

$$e = e_L + e_N \quad (6.37)$$

where the Taylor series of $e = \ln \sqrt{C_{11}}$ has been used to extract its linear and nonlinear parts of displacement, they being

$$e_L = \frac{\partial u}{\partial x} \quad (6.38a)$$

$$e_N = -\frac{1}{2} \frac{\partial u}{\partial x} \frac{\partial u}{\partial x} \quad (6.38b)$$

which have been truncated after their quadratic contribution.

The linear strain-displacement matrix \mathbf{B}_L can now be obtained from the derivatives of displacement as follows

$$e_L = \partial u / \partial x = \sum_{i=1}^2 N_{i,x} u_i = [[\mathbf{b}_{L1}], [\mathbf{b}_{L2}]] \{\Delta\} = [\mathbf{B}_L] \{\Delta\} \quad (6.39a)$$

with

$$\mathbf{b}_{Li} = N_{i,x} \quad \text{and} \quad \Delta^T = \{u_1, u_2\} \quad (6.39b)$$

where u_1 and u_2 are the displacements at the ends of the chord. Furthermore, the nonlinear strain term can be written as

$$e_N = \frac{1}{2} [-\partial u / \partial x] \{\partial u / \partial x\} = \frac{1}{2} \mathbf{A} \boldsymbol{\theta} \quad (6.40)$$

where the derivatives of displacement can be related to the nodal parameters via

$$\boldsymbol{\theta} = \{\partial u / \partial x\} = \{\sum_{i=1}^2 N_{i,x} u_i\} = [[\mathbf{h}_1], [\mathbf{h}_2]] \{\Delta\} = [\mathbf{H}] \{\Delta\} \quad \text{with} \quad \mathbf{h}_i = N_{i,x} \quad (6.41)$$

hence \mathbf{B}_N become

$$\mathbf{B}_N = \mathbf{A} \mathbf{H} = [[\mathbf{b}_{N1}], [\mathbf{b}_{N2}]] \quad (6.42)$$

where

$$\mathbf{b}_{Ni} = [-\partial u / \partial x] \cdot N_{i,x} \quad (6.43)$$

The stress stiffness matrix \mathbf{K}_S expresses the influence of stress on the axial deflection of a chord independent of material properties, specifically

$$\mathbf{K}_S = \int_{\Gamma} \mathbf{H}^T d\mathbf{A}^T \mathbf{T} A dx = \int_{-1}^1 \mathbf{H}^T \mathbf{T} \mathbf{H} \mathbf{J} A d\xi = \sum_{i=1}^n \mathbf{H}^T \mathbf{T} \mathbf{H} \mathbf{J} A w_i \quad (6.44)$$

wherein \mathbf{T} is the stress carried by collagen and elastin fibers, as discussed in Part 4, and \mathbf{H} can be expressed as follows

$$\mathbf{H} = [N_{1,x} \ N_{2,x}] = [N_{1,\xi} \ N_{2,\xi}] \mathbf{J}^{-1} \quad (6.45)$$

where the Jacobian \mathbf{J} is defined in Eqn. 6.9.

The small displacement stiffness matrix for a 1-D alveolar chord that is transformed from global co-ordinate system to the natural coordinate system by the determinant of the Jacobian matrix, i.e., Eq. (6.9) is evaluated numerically as

$$\mathbf{K}_L = \int_{\Gamma} \mathbf{B}_L^T \mathbf{M} \mathbf{B}_L A dx = \int_{-1}^1 \mathbf{B}_L^T \mathbf{M} \mathbf{B}_L \mathbf{J} A d\xi = \sum_{i=1}^n \mathbf{B}_L^T \mathbf{M} \mathbf{B}_L \mathbf{J} A w_i \quad (6.46)$$

with w_i being the weighting coefficients of the Gauss integration rule, and A being the cross section area of alveolar chord. The values of ξ and w_i for $n = 1, 2$, and 3 Gauss integration points are demonstrated in Table 5.1. In calculation of the stiffness matrix for an element, the linear strain-displacement matrix \mathbf{B}_L is required that is the derivatives of the shape functions with respect to the global co-ordinate system

$$\mathbf{B}_L = [N_{1,x} \ N_{2,x}] = [N_{1,\xi} \ N_{2,\xi}] \mathbf{J}^{-1} \quad (6.47)$$

wherein ξ is abscissae of the Gauss integration rule.

The large displacement stiffness matrix for chord can be presented as follow

$$\mathbf{K}_N = \int_{-1}^1 \mathbf{D} \mathbf{J} A d\xi = \sum_{i=1}^n \mathbf{D} \mathbf{J} A w_i \quad (6.48)$$

where \mathbf{D} take the form of

$$\mathbf{D} = \mathbf{B}_L^T \mathbf{M} \mathbf{B}_N + \mathbf{B}_N^T \mathbf{M} \mathbf{B}_L + \mathbf{B}_N^T \mathbf{M} \mathbf{B}_N \quad (6.49)$$

wherein \mathbf{B}_N have the expression

$$\mathbf{B}_N = [\partial \mathbf{u} / \partial \mathbf{x}] [N_{1,x} \ N_{2,x}] = [\sum_{i=1}^n N_{i,x} u_i] [N_{1,\xi} \ N_{2,\xi}] \mathbf{J}^{-1} \quad (6.50)$$

Thereby the total stiffness matrix \mathbf{K}_T can be obtained by summation of stress stiffness matrix, small and large displacement stiffness matrices.

6.2.2. Stiffness Matrix for Pentagon

The components of Laplace stretch \mathcal{U} associated with a planar membrane has a Cholesky factorization expressed in terms of the right Cauchy-Green deformation tensor $\mathbf{C} := \mathbf{F}^T \mathbf{F} = \mathbf{U}^T \mathbf{U}$, which is a symmetric second-order tensor.

$$\begin{aligned} \mathcal{U}_{11} &= \sqrt{C_{11}} & \mathcal{U}_{12} &= C_{12}/\mathcal{U}_{11} \\ \mathcal{U}_{21} &= 0 & \mathcal{U}_{22} &= \sqrt{C_{22} - (\mathcal{U}_{12})^2} \end{aligned} \quad (6.51)$$

where C_{11} , C_{12} , C_{21} and C_{22} are components of the Green deformation matrix \mathbf{C} wherein \mathbf{F} is the deformation gradient.

$$\mathbf{C} = \mathbf{F}^T \mathbf{F} = \begin{bmatrix} C_{11} & C_{12} \\ C_{12} & C_{22} \end{bmatrix} \quad , \quad \mathbf{F} = \begin{bmatrix} 1 + \partial u / \partial x & \partial u / \partial y \\ \partial v / \partial x & 1 + \partial v / \partial y \end{bmatrix} \quad (6.52a)$$

with

$$C_{11} = \left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial x} \right)^2 + 2 \frac{\partial u}{\partial x} + 1 \quad (6.52b)$$

$$C_{12} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} + \frac{\partial u}{\partial x} \cdot \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \cdot \frac{\partial v}{\partial y} \quad (6.52c)$$

$$C_{22} = \left(\frac{\partial u}{\partial y} \right)^2 + \left(\frac{\partial v}{\partial y} \right)^2 + 2 \frac{\partial v}{\partial y} + 1 \quad (6.52d)$$

It is useful to define the total virtual strains Eq. (??) in terms of linear and nonlinear incremental strains as follow

$$\xi = \xi_L + \xi_{N1} + \xi_{N2} \quad (6.53a)$$

$$\varepsilon = \varepsilon_L + \varepsilon_{N1} + \varepsilon_{N2} \quad (6.53b)$$

$$\gamma = \gamma_L + \gamma_{N1} + \gamma_{N2} \quad (6.53c)$$

Taylor series are used here to obtain the linear and nonlinear part of displacements

$$\xi_L = \frac{1}{2} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \quad (6.54a)$$

$$\xi_N = \frac{1}{4} \left(-\frac{\partial v}{\partial y} \frac{\partial v}{\partial y} - \frac{\partial u}{\partial x} \frac{\partial u}{\partial x} - 2 \frac{\partial u}{\partial y} \frac{\partial v}{\partial x} \right) \quad (6.54b)$$

$$\varepsilon_L = \frac{1}{2} \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right) \quad (6.54c)$$

$$\varepsilon_N = \frac{1}{4} \left(2 \frac{\partial v}{\partial x} \frac{\partial v}{\partial x} + \frac{\partial v}{\partial y} \frac{\partial v}{\partial y} - \frac{\partial u}{\partial x} \frac{\partial u}{\partial x} + 2 \frac{\partial u}{\partial y} \frac{\partial v}{\partial x} \right) \quad (6.54d)$$

$$\gamma_L = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \quad (6.54e)$$

$$\gamma_N = \frac{\partial v}{\partial x} \frac{\partial v}{\partial y} - 2 \frac{\partial u}{\partial x} \frac{\partial v}{\partial x} - \frac{\partial u}{\partial x} \frac{\partial u}{\partial y} \quad (6.54f)$$

The linear strain displacement matrix \mathbf{B}_L can be obtained by differentiation of displacements expressed through the nodal displacements and shape functions from infinitesimal linear strain vector that take the form of

$$\begin{aligned} \mathbf{E}_L &= \begin{Bmatrix} \xi_L \\ \varepsilon_L \\ \gamma_L \end{Bmatrix} = \begin{Bmatrix} \frac{1}{2} u_{,x} + \frac{1}{2} v_{,y} \\ \frac{1}{2} u_{,x} - \frac{1}{2} v_{,y} \\ u_{,y} + v_{,x} \end{Bmatrix} = \begin{bmatrix} \frac{1}{2} \sum_{i=1}^5 N_{i,x} & \frac{1}{2} \sum_{i=1}^5 N_{i,y} \\ \frac{1}{2} \sum_{i=1}^5 N_{i,x} & -\frac{1}{2} \sum_{i=1}^5 N_{i,y} \\ \sum_{i=1}^5 N_{i,y} & \sum_{i=1}^5 N_{i,x} \end{bmatrix} \begin{Bmatrix} u_i \\ v_i \end{Bmatrix} \\ &= [[\mathbf{b}_{L1}], [\mathbf{b}_{L2}], [\mathbf{b}_{L3}], [\mathbf{b}_{L4}], [\mathbf{b}_{L5}]] \{\Delta\} = [\mathbf{B}_L] \{\Delta\} \end{aligned} \quad (6.55)$$

wherein

$$\mathbf{b}_{Li} = \begin{bmatrix} \frac{1}{2} N_{i,x} & \frac{1}{2} N_{i,y} \\ \frac{1}{2} N_{i,x} & -\frac{1}{2} N_{i,y} \\ N_{i,y} & N_{i,x} \end{bmatrix} \quad (6.56a)$$

and

$$\Delta^T = \{u_1, v_1, u_2, v_2, \dots, u_n, v_n\} \quad (6.56b)$$

The first nonlinear strain terms can be written as

$$\mathbf{E}_{N1} = \begin{Bmatrix} \xi_{N1} \\ \varepsilon_{N1} \\ \gamma_{N1} \end{Bmatrix} = \begin{Bmatrix} -\frac{1}{4}u_{,x}^2 - \frac{1}{4}v_{,y}^2 \\ -\frac{1}{4}u_{,x}^2 + \frac{1}{4}v_{,y}^2 \\ -u_{,y}u_{,x} + v_{,x}v_{,y} \end{Bmatrix} = \frac{1}{2} \begin{bmatrix} -\frac{1}{2}\partial u/\partial x & -\frac{1}{2}\partial v/\partial y \\ -\frac{1}{2}\partial u/\partial x & \frac{1}{2}\partial v/\partial y \\ -2\partial u/\partial y & 2\partial v/\partial x \end{bmatrix} \begin{Bmatrix} \partial u/\partial x \\ \partial v/\partial y \end{Bmatrix} = \frac{1}{2} [\mathbf{A}_{N1}] [\boldsymbol{\theta}_{N1}] \quad (6.57)$$

the derivative of displacement can be related to the nodal parameters via

$$[\boldsymbol{\theta}_{N1}] = \begin{Bmatrix} \partial u/\partial x \\ \partial v/\partial y \end{Bmatrix} = \begin{Bmatrix} \sum_{i=1}^5 N_{i,x} u_i \\ \sum_{i=1}^5 N_{i,y} v_i \end{Bmatrix} = [[\mathbf{h}_{N1}], [\mathbf{h}_{N2}], [\mathbf{h}_{N3}], [\mathbf{h}_{N4}], [\mathbf{h}_{N5}]] \{\Delta\} = [\mathbf{H}_{N1}] \{\Delta\} \quad (6.58)$$

where

$$\mathbf{h}_{Ni} = \begin{bmatrix} N_{i,x} & 0 \\ 0 & N_{i,y} \end{bmatrix} \quad (6.59)$$

hence \mathbf{B}_{N1} become

$$\mathbf{B}_{N1} = [\mathbf{A}_{N1}] [\mathbf{H}_{N1}] = [[\mathbf{b}_{N1}], [\mathbf{b}_{N2}], [\mathbf{b}_{N3}], [\mathbf{b}_{N4}], [\mathbf{b}_{N5}]] \quad (6.60)$$

where

$$\mathbf{b}_{Ni} = \begin{bmatrix} -\frac{1}{2}\partial u/\partial x & -\frac{1}{2}\partial v/\partial y \\ -\frac{1}{2}\partial u/\partial x & \frac{1}{2}\partial v/\partial y \\ -2\partial u/\partial y & 2\partial v/\partial x \end{bmatrix} \begin{bmatrix} N_{i,x} & 0 \\ 0 & N_{i,y} \end{bmatrix} \quad (6.61)$$

The second nonlinear strain terms can be written as

$$\mathbf{E}_{N2} = \begin{Bmatrix} \xi_{N2} \\ \varepsilon_{N2} \\ \gamma_{N2} \end{Bmatrix} = \begin{Bmatrix} -\frac{1}{2}u_{,y}v_{,x} \\ \frac{1}{2}u_{,y}v_{,x} + \frac{1}{2}v_{,x}^2 \\ -2u_{,x}v_{,x} \end{Bmatrix} = \frac{1}{2} \begin{bmatrix} -\partial v/\partial x & 0 \\ \partial v/\partial x & \partial v/\partial x \\ 0 & -4\partial u/\partial x \end{bmatrix} \begin{Bmatrix} \partial u/\partial y \\ \partial v/\partial x \end{Bmatrix} = \frac{1}{2} [\mathbf{A}_{N2}] [\boldsymbol{\theta}_{N2}] \quad (6.62)$$

the derivative of displacement can be related to the nodal parameters via

$$[\boldsymbol{\theta}_{N2}] = \begin{Bmatrix} \partial u/\partial y \\ \partial v/\partial x \end{Bmatrix} = \begin{Bmatrix} \sum_{i=1}^5 N_{i,y} u_i \\ \sum_{i=1}^5 N_{i,x} v_i \end{Bmatrix} = [[\mathbf{h}_{N1}], [\mathbf{h}_{N2}], [\mathbf{h}_{N3}], [\mathbf{h}_{N4}], [\mathbf{h}_{N5}]] \{\Delta\} = [\mathbf{H}_2] \{\Delta\} \quad (6.63)$$

where

$$\mathbf{h}_{Ni} = \begin{bmatrix} N_{i,y} & 0 \\ 0 & N_{i,x} \end{bmatrix} \quad (6.64)$$

hence \mathbf{B}_{N2} become

$$\mathbf{B}_{N2} = [\mathbf{A}_{N2}] [\mathbf{H}_{N2}] = [[\mathbf{b}_{N1}], [\mathbf{b}_{N2}], [\mathbf{b}_{N3}], [\mathbf{b}_{N4}], [\mathbf{b}_{N5}]] \quad (6.65)$$

where

$$\mathbf{b}_{Ni} = \begin{bmatrix} -\partial v/\partial x & 0 \\ \partial v/\partial x & -\partial v/\partial x \\ 0 & -4\partial u/\partial x \end{bmatrix} \begin{bmatrix} N_{i,y} & 0 \\ 0 & N_{i,x} \end{bmatrix} \quad (6.66)$$

In order to be able to evaluate the nonlinear stiffness matrix, $[\bar{\mathbf{B}}]$ should be established as the summation of \mathbf{B}_{N1} and \mathbf{B}_{N2} . Hence, the stress stiffness matrix for a 2-D alveolar septa take the form of

$$\mathbf{K}_S = \int_{\triangle} \int_{\triangle} d\mathbf{B}_N^T \mathbf{T} |\mathbf{J}| h d\xi d\eta = \sum_{i=1}^n \sum_{j=1}^n d\mathbf{B}_N^T \mathbf{T} |\mathbf{J}| h w_i w_j \quad (6.67)$$

where n stands for number of Gauss points, w_i and w_j denote the natural weight of the element demonstrated in Table 5.3 By taking the variation of Eq. (6.29) and substituting the definition of first and second nonlinear strain displacement matrices, the total nonlinear strain displacement matrix becomes

$$d[\mathbf{B}_N]^T = [\mathbf{H}_{N1}^T]d[\mathbf{A}_{N1}^T] + [\mathbf{H}_{N2}^T]d[\mathbf{A}_{N2}^T] \quad (6.68)$$

which on substituting into Eq. (6.67) gives

$$\mathbf{K}_S d\Delta = \int_A ([\mathbf{H}_1^T]d[\mathbf{A}_1^T] + [\mathbf{H}_2^T]d[\mathbf{A}_2^T]) \begin{Bmatrix} s^\pi \\ s^\sigma \\ s^\tau \end{Bmatrix} dA \quad (6.69)$$

However, using the mathematical properties of the matrix \mathbf{A} , the following expression will appear

$$d[\mathbf{A}_1^T] \begin{Bmatrix} s^\pi \\ s^\sigma \\ s^\tau \end{Bmatrix} = \begin{bmatrix} s^\pi & s^\tau \\ s^\tau & s^\sigma \end{bmatrix} [\mathbf{H}_1] d\Delta \quad \text{and} \quad d[\mathbf{A}_2^T] \begin{Bmatrix} s^\pi \\ s^\sigma \\ s^\tau \end{Bmatrix} = \begin{bmatrix} s^\pi & s^\tau \\ s^\tau & s^\sigma \end{bmatrix} [\mathbf{H}_2] d\Delta \quad (6.70)$$

and finally the stress/geometric stiffness matrix can be expressed as follow

$$\begin{aligned} \mathbf{K}_S &= \int_A [\mathbf{H}_1]^T \begin{bmatrix} s^\pi & s^\tau \\ s^\tau & s^\sigma \end{bmatrix} [\mathbf{H}_1] dA + \int_A [\mathbf{H}_2]^T \begin{bmatrix} s^\pi & s^\tau \\ s^\tau & s^\sigma \end{bmatrix} [\mathbf{H}_2] dA \\ &= \sum_{i=1}^n \sum_{j=1}^n \left([\mathbf{H}_1]^T \begin{bmatrix} s^\pi & s^\tau \\ s^\tau & s^\sigma \end{bmatrix} [\mathbf{H}_1] |\mathbf{J}| h + [\mathbf{H}_2]^T \begin{bmatrix} s^\pi & s^\tau \\ s^\tau & s^\sigma \end{bmatrix} [\mathbf{H}_2] |\mathbf{J}| h \right) w_i w_j \end{aligned} \quad (6.71)$$

The small/linear displacement stiffness matrix for pentagon is evaluated numerically as

$$\mathbf{K}_L = \int_{\triangle} \int_{\triangle} \mathbf{B}_L^T \mathbf{M} \mathbf{B}_L |\mathbf{J}| h d\xi d\eta = \sum_{i=1}^n \sum_{j=1}^n \mathbf{B}_L^T \mathbf{M} \mathbf{B}_L |\mathbf{J}| h w_i w_j \quad (6.72)$$

The large/nonlinear displacement stiffness matrix for chord can be presented as follow

$$\mathbf{K}_N = \int_{\triangle} \int_{\triangle} \mathbf{D} |\mathbf{J}| h d\xi d\eta = \sum_{i=1}^n \sum_{j=1}^n \mathbf{D} |\mathbf{J}| h w_i w_j \quad (6.73)$$

where \mathbf{D} have the expression

$$\mathbf{D} = \mathbf{B}_L^T \mathbf{M} \mathbf{B}_N + \mathbf{B}_N^T \mathbf{M} \mathbf{B}_L + \mathbf{B}_N^T \mathbf{M} \mathbf{B}_N \quad (6.74)$$

6.2.3. Stiffness Matrix for a tetrahedron

The Laplace stretch associated with a alveolar volume has geometric interpretations that one can assign [50]

$$\mathcal{U}_{ij} = \begin{bmatrix} a & a\gamma & a\beta \\ 0 & b & ba \\ 0 & 0 & c \end{bmatrix} \quad (6.75a)$$

The components of Laplace stretch \mathbf{U} has a Cholesky factorization expressed in terms of the right Cauchy-Green deformation tensor $\mathbf{C} := \mathbf{F}^\top \mathbf{F} = \mathbf{U}^\top \mathbf{U}$, which is a symmetric second-order tensor.

$$\begin{aligned} \mathcal{U}_{11} &= \sqrt{C_{11}} & \mathcal{U}_{12} &= C_{12}/\mathcal{U}_{11} & \mathcal{U}_{13} &= C_{13}/\mathcal{U}_{11} \\ \mathcal{U}_{21} &= 0 & \mathcal{U}_{22} &= \sqrt{C_{22} - \mathcal{U}_{12}^2} & \mathcal{U}_{23} &= (C_{23} - \mathcal{U}_{12}\mathcal{U}_{13})/\mathcal{U}_{22} \\ \mathcal{U}_{31} &= 0 & \mathcal{U}_{32} &= 0 & \mathcal{U}_{33} &= \sqrt{C_{33} - \mathcal{U}_{13}^2 - \mathcal{U}_{23}^2} \end{aligned} \quad (6.76)$$

where C_{11}, C_{12}, C_{21} and C_{22} are components of the Green deformation matrix \mathbf{C} wherein \mathbf{F} is the deformation gradient.

$$\mathbf{C} = \mathbf{F}^\top \mathbf{F} = \begin{bmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} 1 + \partial u / \partial x & \partial u / \partial y & \partial u / \partial z \\ \partial v / \partial x & 1 + \partial v / \partial y & \partial v / \partial z \\ \partial w / \partial x & \partial w / \partial y & 1 + \partial w / \partial z \end{bmatrix} \quad (6.77a)$$

with

$$C_{11} = \left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial x} \right)^2 + \left(\frac{\partial w}{\partial x} \right)^2 + 2 \frac{\partial u}{\partial x} + 1 \quad (6.77b)$$

$$C_{22} = \left(\frac{\partial u}{\partial y} \right)^2 + \left(\frac{\partial v}{\partial y} \right)^2 + \left(\frac{\partial w}{\partial y} \right)^2 + 2 \frac{\partial v}{\partial y} + 1 \quad (6.77c)$$

$$C_{33} = \left(\frac{\partial u}{\partial z} \right)^2 + \left(\frac{\partial v}{\partial z} \right)^2 + \left(\frac{\partial w}{\partial z} \right)^2 + 2 \frac{\partial w}{\partial z} + 1 \quad (6.77d)$$

$$C_{12} = C_{21} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} + \frac{\partial u}{\partial x} \cdot \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \cdot \frac{\partial v}{\partial y} + \frac{\partial w}{\partial x} \cdot \frac{\partial w}{\partial y} \quad (6.77e)$$

$$C_{13} = C_{31} = \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} + \frac{\partial u}{\partial x} \cdot \frac{\partial u}{\partial z} + \frac{\partial v}{\partial x} \cdot \frac{\partial v}{\partial z} + \frac{\partial w}{\partial x} \cdot \frac{\partial w}{\partial z} \quad (6.77f)$$

$$C_{23} = C_{32} = \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} + \frac{\partial u}{\partial y} \cdot \frac{\partial u}{\partial z} + \frac{\partial v}{\partial y} \cdot \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \cdot \frac{\partial w}{\partial z} \quad (6.77g)$$

the dilatation δ for the alveolar volume is

$$\xi := \ln \sqrt[3]{\frac{a}{a_0} \frac{b}{b_0} \frac{c}{c_0}} \quad (6.78a)$$

and the squeezes ε_i and the shear strains γ_i are defined accordingly

$$\varepsilon_1 := \ln \sqrt[3]{\frac{a}{a_0} \frac{b_0}{b}} \quad \gamma_1 := \alpha - \alpha_0 \quad (6.78b)$$

$$\varepsilon_2 := \ln \sqrt[3]{\frac{b}{b_0} \frac{c_0}{c}} \quad \gamma_2 := \beta - \beta_0 \quad (6.78c)$$

$$\varepsilon_3 := \ln \sqrt[3]{\frac{c}{c_0} \frac{a_0}{a}} \quad \gamma_3 := \gamma - \gamma_0 \quad (6.78d)$$

wherein a_0 , b_0 and c_0 are their initial elongation ratios, and where α_0 , β_0 and γ_0 are their initial shears. It is useful to define the above strains in terms of linear and nonlinear incremental strains as follow

$$\xi = \xi_L + \xi_{N1} + \xi_{N2} + \xi_{N3} \quad (6.79a)$$

$$\varepsilon_i = \varepsilon_{iL} + \varepsilon_{iN1} + \varepsilon_{iN2} + \varepsilon_{iN3} \quad (6.79b)$$

$$\gamma_i = \gamma_{iL} + \gamma_{iN1} + \gamma_{iN2} + \gamma_{iN3} \quad (6.79c)$$

Taylor series are used here to obtain the linear and nonlinear part of displacements

$$\xi_L = \frac{1}{3} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \quad (6.80a)$$

$$\begin{aligned} \xi_N = & \frac{1}{6} \left(-\frac{\partial u}{\partial x} \frac{\partial u}{\partial x} + \frac{\partial u}{\partial z} \frac{\partial u}{\partial z} - \frac{\partial v}{\partial y} \frac{\partial v}{\partial y} - \frac{\partial v}{\partial z} \frac{\partial v}{\partial z} + \frac{\partial w}{\partial x} \frac{\partial w}{\partial x} - \frac{\partial w}{\partial y} \frac{\partial w}{\partial y} - \frac{\partial w}{\partial z} \frac{\partial w}{\partial z} \right. \\ & \left. - 2 \frac{\partial u}{\partial y} \frac{\partial v}{\partial x} - 4 \frac{\partial v}{\partial z} \frac{\partial w}{\partial y} \right) \end{aligned} \quad (6.80b)$$

$$\varepsilon_{1L} = \frac{1}{3} \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right) \quad (6.80c)$$

$$\varepsilon_{1N} = \frac{1}{6} \left(2 \frac{\partial v}{\partial x} \frac{\partial v}{\partial x} + \frac{\partial v}{\partial y} \frac{\partial v}{\partial y} - \frac{\partial u}{\partial x} \frac{\partial u}{\partial x} + \frac{\partial w}{\partial x} \frac{\partial w}{\partial x} - \frac{\partial w}{\partial y} \frac{\partial w}{\partial y} + 2 \frac{\partial u}{\partial y} \frac{\partial v}{\partial x} \right) \quad (6.80d)$$

$$\varepsilon_{2L} = \frac{1}{3} \left(\frac{\partial v}{\partial y} - \frac{\partial w}{\partial z} \right) \quad (6.80e)$$

$$\begin{aligned} \varepsilon_{2N} = & \frac{1}{6} \left(-\frac{\partial v}{\partial x} \frac{\partial v}{\partial x} - \frac{\partial v}{\partial y} \frac{\partial v}{\partial y} - \frac{\partial u}{\partial z} \frac{\partial u}{\partial z} + \frac{\partial v}{\partial z} \frac{\partial v}{\partial z} + 3 \frac{\partial w}{\partial y} \frac{\partial w}{\partial y} + \frac{\partial w}{\partial z} \frac{\partial w}{\partial z} \right. \\ & \left. - 2 \frac{\partial u}{\partial y} \frac{\partial v}{\partial x} + 4 \frac{\partial v}{\partial z} \frac{\partial w}{\partial y} \right) \end{aligned} \quad (6.80f)$$

$$\varepsilon_{3L} = \frac{1}{3} \left(-\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} \right) \quad (6.80g)$$

$$\begin{aligned} \varepsilon_{3N} = & \frac{1}{6} \left(-\frac{\partial v}{\partial x} \frac{\partial v}{\partial x} + \frac{\partial u}{\partial x} \frac{\partial u}{\partial x} + \frac{\partial u}{\partial z} \frac{\partial u}{\partial z} - \frac{\partial v}{\partial z} \frac{\partial v}{\partial z} - \frac{\partial w}{\partial x} \frac{\partial w}{\partial x} - 2 \frac{\partial w}{\partial y} \frac{\partial w}{\partial y} \right. \\ & \left. - \frac{\partial w}{\partial z} \frac{\partial w}{\partial z} - 4 \frac{\partial v}{\partial z} \frac{\partial w}{\partial y} \right) \end{aligned} \quad (6.80h)$$

$$\gamma_{1L} = \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \quad (6.80i)$$

$$\begin{aligned} \gamma_{1N} = & 2 \frac{\partial u}{\partial x} \frac{\partial v}{\partial z} - \frac{\partial u}{\partial z} \frac{\partial v}{\partial x} + 2 \frac{\partial u}{\partial x} \frac{\partial w}{\partial y} - \frac{\partial u}{\partial y} \frac{\partial w}{\partial x} - \frac{\partial v}{\partial y} \frac{\partial v}{\partial z} - \frac{\partial v}{\partial x} \frac{\partial w}{\partial x} \\ & - 2 \frac{\partial v}{\partial y} \frac{\partial w}{\partial z} + \frac{\partial w}{\partial y} \frac{\partial w}{\partial z} \end{aligned} \quad (6.80j)$$

$$\gamma_{2L} = \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \quad (6.80k)$$

$$\gamma_{2N} = \frac{\partial u}{\partial y} \frac{\partial u}{\partial z} - 2 \frac{\partial u}{\partial x} \frac{\partial v}{\partial z} - 2 \frac{\partial u}{\partial x} \frac{\partial w}{\partial y} + \frac{\partial v}{\partial y} \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \frac{\partial w}{\partial z} \quad (6.80l)$$

$$\gamma_{3L} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \quad (6.80m)$$

$$\gamma_{3N} = -\frac{\partial u}{\partial x} \frac{\partial u}{\partial y} - 2 \frac{\partial u}{\partial x} \frac{\partial v}{\partial x} + \frac{\partial v}{\partial x} \frac{\partial v}{\partial y} + \frac{\partial w}{\partial x} \frac{\partial w}{\partial y} \quad (6.80n)$$

The linear strain displacement matrix \mathbf{B}_L can be obtained by differentiation of displacements expressed through the nodal displacements and shape functions from infinitesimal linear

strain vector that take the form of

$$\mathbf{E}_L = \begin{Bmatrix} \xi_L \\ \varepsilon_{1L} \\ \varepsilon_{2L} \\ \varepsilon_{3L} \\ \gamma_{1L} \\ \gamma_{2L} \\ \gamma_{3L} \end{Bmatrix} = \begin{Bmatrix} \frac{1}{3} u_{,x} + \frac{1}{3} v_{,y} + \frac{1}{3} w_{,z} \\ \frac{1}{3} u_{,x} - \frac{1}{3} v_{,y} \\ \frac{1}{3} v_{,y} - \frac{1}{3} w_{,z} \\ -\frac{1}{3} u_{,x} + \frac{1}{3} w_{,z} \\ v_{,z} + w_{,y} \\ v_{,z} + w_{,y} \\ u_{,y} + v_{,x} \end{Bmatrix} = \begin{Bmatrix} \frac{1}{3} \sum_{i=1}^4 N_{i,x} & \frac{1}{3} \sum_{i=1}^4 N_{i,y} & \frac{1}{3} \sum_{i=1}^4 N_{i,z} \\ \frac{1}{3} \sum_{i=1}^4 N_{i,x} & \frac{-1}{3} \sum_{i=1}^4 N_{i,y} & 0 \\ 0 & \frac{1}{3} \sum_{i=1}^4 N_{i,y} & \frac{-1}{3} \sum_{i=1}^4 N_{i,z} \\ \frac{-1}{3} \sum_{i=1}^4 N_{i,x} & 0 & \frac{1}{3} \sum_{i=1}^4 N_{i,z} \\ 0 & \sum_{i=1}^4 N_{i,z} & \frac{1}{3} \sum_{i=1}^4 N_{i,y} \\ 0 & \sum_{i=1}^4 N_{i,z} & \sum_{i=1}^4 N_{i,y} \\ \sum_{i=1}^4 N_{i,y} & \sum_{i=1}^4 N_{i,x} & 0 \end{Bmatrix} \begin{Bmatrix} u_i \\ v_i \\ w_i \end{Bmatrix}$$

$$= [[\mathbf{b}_{L1}], [\mathbf{b}_{L2}], [\mathbf{b}_{L3}], [\mathbf{b}_{L4}]] \{\Delta\} = [\mathbf{B}_L] \{\Delta\} \quad (6.81)$$

wherein

$$\mathbf{b}_{Li} = \begin{Bmatrix} \frac{1}{3} N_{i,x} & \frac{1}{3} N_{i,y} & \frac{1}{3} N_{i,z} \\ \frac{1}{3} N_{i,x} & -\frac{1}{3} N_{i,y} & 0 \\ 0 & \frac{1}{3} N_{i,y} & -\frac{1}{3} N_{i,z} \\ -\frac{1}{3} N_{i,x} & 0 & \frac{1}{3} N_{i,z} \\ 0 & N_{i,z} & N_{i,y} \\ 0 & N_{i,z} & N_{i,y} \\ N_{i,y} & N_{i,x} & 0 \end{Bmatrix} \quad (6.82a)$$

and

$$\Delta^T = \{u_1, v_1, w_1, u_2, v_2, w_2, \dots, u_n, v_n, w_n\} \quad (6.82b)$$

The first nonlinear strain terms can be written as

$$\mathbf{E}_{N1} = \begin{Bmatrix} \xi_L \\ \varepsilon_{1N} \\ \varepsilon_{2N} \\ \varepsilon_{3N} \\ \gamma_{1N} \\ \gamma_{2N} \\ \gamma_{3N} \end{Bmatrix} = \begin{Bmatrix} \frac{1}{6} (-u_{,x}^2 - 2u_{,y}v_{,x} + w_{,x}^2) \\ \frac{1}{6} (-u_{,x}^2 + 2v_{,x}^2 + w_{,x}^2) \\ \frac{1}{6} (-v_{,x}^2) \\ \frac{1}{6} (u_{,x}^2 - v_{,x}^2 - w_{,x}^2) \\ 2u_{,x}v_{,z} - u_{,z}v_{,x} - v_{,x}w_{,x} \\ -2u_{,x}v_{,z} \\ -u_{,x}u_{,y} - 2u_{,x}v_{,x} \end{Bmatrix}$$

$$= \frac{1}{2} \begin{Bmatrix} -\frac{1}{3} \partial u / \partial x & -\frac{2}{3} \partial u / \partial y & \frac{1}{3} \partial w / \partial x \\ -\frac{1}{3} \partial u / \partial x & \frac{2}{3} \partial v / \partial x & \frac{1}{3} \partial w / \partial x \\ 0 & -\frac{1}{3} \partial v / \partial x & 0 \\ \frac{1}{3} \partial u / \partial x & -\frac{1}{3} \partial v / \partial x & -\frac{1}{3} \partial w / \partial x \\ 4 \partial v / \partial z & -2 \partial u / \partial z & -2 \partial v / \partial x \\ -4 \partial v / \partial z & 0 & 0 \\ -2 \partial u / \partial y & -4 \partial u / \partial x & 0 \end{Bmatrix} \begin{Bmatrix} \partial u / \partial x \\ \partial v / \partial x \\ \partial w / \partial x \end{Bmatrix} = \frac{1}{2} [\mathbf{A}_{N1}] [\boldsymbol{\theta}_{N1}] \quad (6.83)$$

the derivative of displacement can be related to the nodal parameters via

$$[\boldsymbol{\theta}_{N1}] = \begin{Bmatrix} \partial u / \partial x \\ \partial v / \partial x \\ \partial w / \partial x \end{Bmatrix} = \begin{Bmatrix} \sum_{i=1}^5 N_{i,x} u_i \\ \sum_{i=1}^5 N_{i,x} v_i \\ \sum_{i=1}^5 N_{i,x} w_i \end{Bmatrix} = [[\mathbf{h}_{N1}], [\mathbf{h}_{N2}], [\mathbf{h}_{N3}], [\mathbf{h}_{N4}]] \{\Delta\} = [\mathbf{H}_{N1}] \{\Delta\} \quad (6.84)$$

where

$$\mathbf{h}_{Ni} = \begin{bmatrix} N_{i,x} & 0 & 0 \\ 0 & N_{i,x} & 0 \\ 0 & 0 & N_{i,x} \end{bmatrix} \quad (6.85)$$

hence \mathbf{B}_{N1} become

$$\mathbf{B}_{N1} = [\mathbf{A}_{N1}] [\mathbf{H}_{N1}] = [[\mathbf{b}_{N1}], [\mathbf{b}_{N2}], [\mathbf{b}_{N3}], [\mathbf{b}_{N4}]] \quad (6.86)$$

where

$$\mathbf{b}_i = \begin{bmatrix} -\frac{1}{3} \partial u / \partial x & -\frac{2}{3} \partial u / \partial y & \frac{1}{3} \partial w / \partial x \\ -\frac{1}{3} \partial u / \partial x & \frac{2}{3} \partial v / \partial x & \frac{1}{3} \partial w / \partial x \\ 0 & -\frac{1}{3} \partial v / \partial x & 0 \\ \frac{1}{3} \partial u / \partial x & -\frac{1}{3} \partial v / \partial x & -\frac{1}{3} \partial w / \partial x \\ 4 \partial v / \partial z & -2 \partial u / \partial z & -2 \partial v / \partial x \\ -4 \partial v / \partial z & 0 & 0 \\ -2 \partial u / \partial y & -4 \partial u / \partial x & 0 \end{bmatrix} \begin{bmatrix} N_{i,x} & 0 & 0 \\ 0 & N_{i,x} & 0 \\ 0 & 0 & N_{i,x} \end{bmatrix} \quad (6.87)$$

The second nonlinear strain terms can be written as

$$\begin{aligned} \mathbf{E}_{N2} &= \begin{Bmatrix} \xi_L \\ \varepsilon_{1N} \\ \varepsilon_{2N} \\ \varepsilon_{3N} \\ \gamma_{1N} \\ \gamma_{2N} \\ \gamma_{3N} \end{Bmatrix} = \begin{Bmatrix} \frac{1}{6} (-v_{,y}^2 - w_{,y}^2) \\ \frac{1}{6} (2u_{,y}v_{,x} + 2v_{,y}^2 - w_{,y}^2) \\ \frac{1}{6} (-2u_{,y}v_{,x} - v_{,y}^2 + 3w_{,y}^2) \\ \frac{1}{6} (-2w_{,y}^2) \\ -u_{,y}w_{,x} - 2v_{,y}w_{,y} + w_{,y}w_{,z} \\ u_{,y}u_{,z} - 2u_{,x}w_{,y} \\ v_{,x}v_{,y} + w_{,x}w_{,y} \end{Bmatrix} \\ &= \frac{1}{2} \begin{bmatrix} 0 & -\frac{1}{3} \partial v / \partial y & \frac{1}{3} \partial w / \partial y \\ \frac{2}{3} \partial v / \partial x & \frac{2}{3} \partial v / \partial y & -\frac{1}{3} \partial w / \partial y \\ -\frac{2}{3} \partial v / \partial x & -\frac{1}{3} \partial v / \partial y & \partial w / \partial y \\ 0 & 0 & -\frac{2}{3} \partial w / \partial y \\ -2 \partial w / \partial x & -4 \partial w / \partial y & 2 \partial w / \partial z \\ 2 \partial u / \partial z & 0 & -4 \partial u / \partial x \\ 0 & 2 \partial v / \partial x & 2 \partial w / \partial x \end{bmatrix} \begin{Bmatrix} \partial u / \partial y \\ \partial v / \partial y \\ \partial w / \partial y \end{Bmatrix} = \frac{1}{2} [\mathbf{A}_{N2}] [\boldsymbol{\theta}_{N2}] \end{aligned} \quad (6.88)$$

the derivative of displacement can be related to the nodal parameters via

$$[\boldsymbol{\theta}_{N2}] = \begin{Bmatrix} \partial u / \partial y \\ \partial v / \partial y \\ \partial w / \partial y \end{Bmatrix} = \begin{Bmatrix} \sum_{i=1}^5 N_{i,y} u_i \\ \sum_{i=1}^5 N_{i,y} v_i \\ \sum_{i=1}^5 N_{i,y} w_i \end{Bmatrix} = [[\mathbf{h}_{N1}], [\mathbf{h}_{N2}], [\mathbf{h}_{N3}], [\mathbf{h}_{N4}]] \{\Delta\} = [\mathbf{H}_{N2}] \{\Delta\} \quad (6.89)$$

where

$$\mathbf{h}_{Ni} = \begin{bmatrix} N_{i,y} & 0 & 0 \\ 0 & N_{i,y} & 0 \\ 0 & 0 & N_{i,y} \end{bmatrix} \quad (6.90)$$

hence \mathbf{B}_{N2} become

$$\mathbf{B}_{N2} = [\mathbf{A}_{N2}] [\mathbf{H}_{N2}] = [[\mathbf{b}_{N1}], [\mathbf{b}_{N2}], [\mathbf{b}_{N3}], [\mathbf{b}_{N4}]] \quad (6.91)$$

where

$$\mathbf{b}_{Ni} = \begin{bmatrix} 0 & -\frac{1}{3} \partial v / \partial y & \frac{1}{3} \partial w / \partial y \\ \frac{2}{3} \partial v / \partial x & \frac{2}{3} \partial v / \partial y & -\frac{1}{3} \partial w / \partial y \\ -\frac{2}{3} \partial v / \partial x & -\frac{1}{3} \partial v / \partial y & \partial w / \partial y \\ 0 & 0 & -\frac{2}{3} \partial w / \partial y \\ -2 \partial w / \partial x & -4 \partial w / \partial y & 2 \partial w / \partial z \\ 2 \partial u / \partial z & 0 & -4 \partial u / \partial x \\ 0 & 2 \partial v / \partial x & 2 \partial w / \partial x \end{bmatrix} \begin{bmatrix} N_{i,y} & 0 & 0 \\ 0 & N_{i,y} & 0 \\ 0 & 0 & N_{i,y} \end{bmatrix} \quad (6.92)$$

The third nonlinear strain terms can be written as

$$\begin{aligned} \mathbf{E}_{N3} &= \begin{Bmatrix} \xi_L \\ \varepsilon_{1N} \\ \varepsilon_{2N} \\ \varepsilon_{3N} \\ \gamma_{1N} \\ \gamma_{2N} \\ \gamma_{3N} \end{Bmatrix} = \begin{Bmatrix} \frac{1}{6} (u_{,z}^2 - v_{,z}^2 - 4v_{,z}w_{,y} - w_{,z}^2) \\ 0 \\ \frac{1}{6} (-u_{,z}^2 + v_{,z}^2 + 4v_{,z}w_{,y} + w_{,z}^2) \\ \frac{1}{6} (u_{,z}^2 - v_{,z}^2 - w_{,z}^2 - 4v_{,z}w_{,y}) \\ -v_{,y}v_{,z} \\ v_{,y}v_{,z} + w_{,y}w_{,z} \\ 0 \end{Bmatrix} \\ &= \frac{1}{2} \begin{bmatrix} \frac{1}{3} \partial u / \partial z & -\frac{1}{3} \partial v / \partial z - \frac{4}{3} \partial w / \partial y & -\frac{1}{3} \partial w / \partial z \\ 0 & 0 & 0 \\ -\frac{1}{3} \partial u / \partial z & \frac{1}{3} \partial v / \partial z + \frac{4}{3} \partial w / \partial y & \frac{1}{3} \partial w / \partial z \\ \frac{1}{3} \partial u / \partial z & -\frac{1}{3} \partial v / \partial z - \frac{4}{3} \partial w / \partial y & -\frac{1}{3} \partial w / \partial z \\ 0 & -2 \partial v / \partial y & 0 \\ 0 & 2 \partial v / \partial y & 2 \partial w / \partial y \\ 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} \partial u / \partial z \\ \partial v / \partial z \\ \partial w / \partial z \end{Bmatrix} = \frac{1}{2} [\mathbf{A}_{N3}] [\boldsymbol{\theta}_{N3}] \end{aligned} \quad (6.93)$$

the derivative of displacement can be related to the nodal parameters via

$$[\boldsymbol{\theta}_{N3}] = \begin{Bmatrix} \partial u / \partial z \\ \partial v / \partial z \\ \partial w / \partial z \end{Bmatrix} = \begin{Bmatrix} \sum_{i=1}^5 N_{i,z} u_i \\ \sum_{i=1}^5 N_{i,z} v_i \\ \sum_{i=1}^5 N_{i,z} w_i \end{Bmatrix} = [[\mathbf{h}_{N1}], [\mathbf{h}_{N2}], [\mathbf{h}_{N3}], [\mathbf{h}_{N4}]] \{\Delta\} = [\mathbf{H}_{N3}] \{\Delta\} \quad (6.94)$$

where

$$\mathbf{h}_{Ni} = \begin{bmatrix} N_{i,z} & 0 & 0 \\ 0 & N_{i,z} & 0 \\ 0 & 0 & N_{i,z} \end{bmatrix} \quad (6.95)$$

hence \mathbf{B}_{N3} become

$$\mathbf{B}_{N3} = [\mathbf{A}_{N3}] [\mathbf{H}_{N3}] = [[\mathbf{b}_{N1}], [\mathbf{b}_{N2}], [\mathbf{b}_{N3}], [\mathbf{b}_{N4}]] \quad (6.96)$$

where

$$\mathbf{b}_{Ni} = \begin{bmatrix} \frac{1}{3} \partial u / \partial z & -\frac{1}{3} \partial v / \partial z - \frac{4}{3} \partial w / \partial y & -\frac{1}{3} \partial w / \partial z \\ 0 & 0 & 0 \\ -\frac{1}{3} \partial u / \partial z & \frac{1}{3} \partial v / \partial z + \frac{4}{3} \partial w / \partial y & \frac{1}{3} \partial w / \partial z \\ \frac{1}{3} \partial u / \partial z & -\frac{1}{3} \partial v / \partial z - \frac{4}{3} \partial w / \partial y & -\frac{1}{3} \partial w / \partial z \\ 0 & -2 \partial v / \partial y & 0 \\ 0 & 2 \partial v / \partial y & 2 \partial w / \partial y \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} N_{i,z} & 0 & 0 \\ 0 & N_{i,z} & 0 \\ 0 & 0 & N_{i,z} \end{bmatrix} \quad (6.97)$$

In order to be able to evaluate the nonlinear stiffness matrix, $[\bar{\mathbf{B}}]$ should be established as the summation of \mathbf{B}_{N1} , \mathbf{B}_{N2} and \mathbf{B}_{N3} . Hence, the stress stiffness matrix for a 3-D alveolar volume take the form of

$$\mathbf{K}_S = \int_V d\mathbf{B}_N^T \mathbf{T} |\mathbf{J}| d\xi d\eta d\zeta = \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^n d\mathbf{B}_N^T \mathbf{T} |\mathbf{J}| w_i w_j w_k \quad (6.98)$$

where n stands for number of Gauss points. Table 5.4 By taking the variation of Eq. (6.29) and substituting the definition of first and second nonlinear strain displacement matrices, the total nonlinear strain displacement matrix becomes

$$d[\mathbf{B}_N]^T = [\mathbf{H}_1^T]d[\mathbf{A}_1^T] + [\mathbf{H}_2^T]d[\mathbf{A}_2^T] + [\mathbf{H}_3^T]d[\mathbf{A}_3^T] \quad (6.99)$$

which on substituting into Eq. (6.98) gives

$$\mathbf{K}_S d\Delta = \int_A ([\mathbf{H}_1^T]d[\mathbf{A}_1^T] + [\mathbf{H}_2^T]d[\mathbf{A}_2^T] + [\mathbf{H}_3^T]d[\mathbf{A}_3^T]) \left\{ \begin{array}{c} s^\pi \\ s^{\sigma_1} \\ s^{\sigma_2} \\ s^{\tau_1} \\ s^{\tau_2} \\ s^{\tau_3} \end{array} \right\} dA \quad (6.100)$$

However, using the mathematical properties of the matrix \mathbf{A} , the following expression will

appear

$$\begin{aligned}
 d[\mathbf{A}_1^T] \begin{Bmatrix} s^\pi \\ s^{\sigma_1} \\ s^{\sigma_2} \\ s^{\tau_1} \\ s^{\tau_2} \\ s^{\tau_3} \end{Bmatrix} &= \begin{bmatrix} s^\pi & s^{\tau_1} & s^{\tau_3} \\ s^{\tau_1} & s^{\sigma_1} & s^{\tau_2} \\ s^{\tau_3} & s^{\tau_2} & s^{\sigma_2} \end{bmatrix} [\mathbf{H}_1] d\Delta \\
 d[\mathbf{A}_2^T] \begin{Bmatrix} s^\pi \\ s^{\sigma_1} \\ s^{\sigma_2} \\ s^{\tau_1} \\ s^{\tau_2} \\ s^{\tau_3} \end{Bmatrix} &= \begin{bmatrix} s^\pi & s^{\tau_1} & s^{\tau_3} \\ s^{\tau_1} & s^{\sigma_1} & s^{\tau_2} \\ s^{\tau_3} & s^{\tau_2} & s^{\sigma_2} \end{bmatrix} [\mathbf{H}_2] d\Delta \\
 d[\mathbf{A}_3^T] \begin{Bmatrix} s^\pi \\ s^{\sigma_1} \\ s^{\sigma_2} \\ s^{\tau_1} \\ s^{\tau_2} \\ s^{\tau_3} \end{Bmatrix} &= \begin{bmatrix} s^\pi & s^{\tau_1} & s^{\tau_3} \\ s^{\tau_1} & s^{\sigma_1} & s^{\tau_2} \\ s^{\tau_3} & s^{\tau_2} & s^{\sigma_3} \end{bmatrix} [\mathbf{H}_3] d\Delta
 \end{aligned} \tag{6.101}$$

and finally the stress/geometric stiffness matrix can be expressed as follow

$$\begin{aligned}
 \mathbf{K}_S = \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^n [\mathbf{H}_1]^T &\begin{bmatrix} s^\pi & s^{\tau_1} & s^{\tau_3} \\ s^{\tau_1} & s^{\sigma_1} & s^{\tau_2} \\ s^{\tau_3} & s^{\tau_2} & s^{\sigma_2} \end{bmatrix} [\mathbf{H}_1] |\mathbf{J}| w_i w_j w_k \\
 + \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^n [\mathbf{H}_2]^T &\begin{bmatrix} s^\pi & s^{\tau_1} & s^{\tau_3} \\ s^{\tau_1} & s^{\sigma_1} & s^{\tau_2} \\ s^{\tau_3} & s^{\tau_2} & s^{\sigma_2} \end{bmatrix} [\mathbf{H}_2] |\mathbf{J}| w_i w_j w_k \\
 + \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^n [\mathbf{H}_3]^T &\begin{bmatrix} s^\pi & s^{\tau_1} & s^{\tau_3} \\ s^{\tau_1} & s^{\sigma_1} & s^{\tau_2} \\ s^{\tau_3} & s^{\tau_2} & s^{\sigma_2} \end{bmatrix} [\mathbf{H}_3] |\mathbf{J}| w_i w_j w_k
 \end{aligned} \tag{6.102}$$

The small/linear displacement stiffness matrix for tetrahedron is evaluated numerically as

$$\mathbf{K}_L = \int_V \mathbf{B}_L^T \mathbf{M} \mathbf{B}_L |\mathbf{J}| d\xi d\eta d\zeta = \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^n \mathbf{B}_L^T \mathbf{M} \mathbf{B}_L |\mathbf{J}| w_i w_j w_k \tag{6.103}$$

The large/nonlinear displacement stiffness matrix for chord can be presented as follow

$$\mathbf{K}_N = \int_V \mathbf{D} |\mathbf{J}| d\xi d\eta d\zeta = \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^n \mathbf{D} |\mathbf{J}| w_i w_j w_k \tag{6.104}$$

where \mathbf{D} have the expression

$$\mathbf{D} = \mathbf{B}_L^T \mathbf{M} \mathbf{B}_N + \mathbf{B}_N^T \mathbf{M} \mathbf{B}_L + \mathbf{B}_N^T \mathbf{M} \mathbf{B}_N \tag{6.105}$$

6.3. Force Vector

The principle of stationary potential energy with the Rayleigh-Ritz approach, Eq. (6.26) determines the basis of finite element stress analysis. The internal strain energy is balanced with the potential energy of applied internal and external loads on the body.

The virtual work done by external forces δW in Eq. (6.26) can be expressed as follow

$$\delta W = \int_S \mathbf{t} \delta \mathbf{u} dS = \int_S \mathbf{t} \mathbf{N} d\Delta dS = \left(\int_S \mathbf{N}^T \mathbf{t} dS \right) d\Delta \quad (6.106)$$

where dS denotes the surface element and \mathbf{t} is the surface traction vector (per unit surface area) at current time. Hence, the external FE force vectors are

$$\mathbf{F} = \int_S \mathbf{N}^T \mathbf{t} dS \quad (6.107)$$

with \mathbf{F} being the deformation gradient.

6.3.1. Force Vector for a Chord

The force vector of the 1-D alveolar chord that is evaluated numerically in its natural co-ordinate system can be described as

$$\mathbf{F}_{1D} = \int_{\Gamma} \mathbf{N}^T \mathbf{t} dx = \int_{-1}^1 \mathbf{N}^T \mathbf{t} \mathbf{J} d\xi = \sum_{i=1}^n \mathbf{N}^T \mathbf{t} \mathbf{J} w_i \quad (6.108)$$

where w_i being the weighting coefficients of the Gauss integration rule, \mathbf{N} is the shape function matrix for chord, and \mathbf{t} is the traction on the septal chord that is selected so that $\mathbf{t} = \mathbf{t}^c + \mathbf{t}^e$ as established in part 4 via engineering stress carried by collagen and elastin fibers. Table 5.1 demonstrates the values of ξ and w_i for $n = 1, 2$, and 3 Gauss integration points.

6.3.2. Force Vector for a Pentagon

The boundary of a two dimensional pentagon consist of line segments, which can be considered as one-dimensional chord. Hence, the evaluation of the boundary integrals on pentagon amounts to evaluating line integrals. Once the interpolation function for a pentagon are evaluated on the boundary of pentagon, we obtain the corresponding chordal interpolation functions [99]. Thus, the force vector \mathbf{F}_{2D} for a pentagon can be obtained by integral over all sides of pentagon as follow

$$\begin{aligned} \mathbf{F}_{2D} &= \oint_{\Gamma} \mathbf{N}^T \mathbf{t} dS = \int_{\Gamma_{12}} \mathbf{N}^T \mathbf{t}_{12} |\mathbf{J}| d\xi + \int_{\Gamma_{23}} \mathbf{N}^T \mathbf{t}_{23} |\mathbf{J}| d\xi + \int_{\Gamma_{34}} \mathbf{N}^T \mathbf{t}_{34} |\mathbf{J}| d\xi \\ &\quad + \int_{\Gamma_{45}} \mathbf{N}^T \mathbf{t}_{45} |\mathbf{J}| d\xi + \int_{\Gamma_{51}} \mathbf{N}^T \mathbf{t}_{51} |\mathbf{J}| d\xi \\ &= \sum_{i=1}^n \mathbf{N}^T \mathbf{t}_{12} |\mathbf{J}| w_i + \sum_{i=1}^n \mathbf{N}^T \mathbf{t}_{23} |\mathbf{J}| w_i + \sum_{i=1}^n \mathbf{N}^T \mathbf{t}_{34} |\mathbf{J}| w_i \\ &\quad + \sum_{i=1}^n \mathbf{N}^T \mathbf{t}_{45} |\mathbf{J}| w_i + \sum_{i=1}^n \mathbf{N}^T \mathbf{t}_{51} |\mathbf{J}| w_i \end{aligned} \quad (6.109)$$

wherein \mathbf{N} being the shape function matrix of a chord with the matrix dimension of a pentagon, $|\mathbf{J}|$ being the determinant of the Jacobian for a 1-D chord, w_i denotes the natural weight of the chord, dS is the arc-length of an infinitesimal line element along the boundary, and \mathbf{t} is the traction vector on each edge of the pentagon as follow

$$\mathbf{t} = \boldsymbol{\sigma}^T \cdot \mathbf{n} \quad (6.110)$$

where \mathbf{n} is the normal vector to each sides of pentagon on which the traction acts and $\boldsymbol{\sigma}$ is the Cauchy stress as established in part 4.

6.3.3. Force Vector for a Tetrahedron

The analysis to find the force vector of a tetrahedron is used to reach the force vector of whole alveolar volume. The matrix of shape functions Eq. (6.20) is used to obtain the force vector for tetrahedron. The force vector \mathbf{F}_{3D} can be specified as follow

$$\begin{aligned} \mathbf{F}_{3D} &= \oint_A \mathbf{N}^T \mathbf{t} dA = \int_{\Delta_1} \int_{\Delta_1} \mathbf{N}^T \mathbf{t}_{\Delta_1} |\mathbf{J}| d\xi d\eta + \int_{\Delta_2} \int_{\Delta_2} \mathbf{N}^T \mathbf{t}_{\Delta_2} |\mathbf{J}| d\xi d\eta \\ &\quad + \int_{\Delta_3} \int_{\Delta_3} \mathbf{N}^T \mathbf{t}_{\Delta_3} |\mathbf{J}| d\xi d\eta + \int_{\Delta_4} \int_{\Delta_4} \mathbf{N}^T \mathbf{t}_{\Delta_4} |\mathbf{J}| d\xi d\eta \\ &= \sum_{i=1}^n \sum_{j=1}^n \mathbf{N}^T \mathbf{t}_{\Delta_1} |\mathbf{J}| w_i w_j + \sum_{i=1}^n \sum_{j=1}^n \mathbf{N}^T \mathbf{t}_{\Delta_2} |\mathbf{J}| w_i w_j \\ &\quad + \sum_{i=1}^n \sum_{j=1}^n \mathbf{N}^T \mathbf{t}_{\Delta_3} |\mathbf{J}| w_i w_j + \sum_{i=1}^n \sum_{j=1}^n \mathbf{N}^T \mathbf{t}_{\Delta_4} |\mathbf{J}| w_i w_j \end{aligned} \quad (6.111)$$

wherein \mathbf{N} being the shape function matrix for a triangle with the matrix dimension of a tetrahedron, $|\mathbf{J}|$ being the determinant of the Jacobian for triangle, n stands for number of Gauss points, w_i and w_j are the natural weight of the triangle from Table 6.1, and \mathbf{t} is the surface traction on the triangle surface. \oint denotes the integral over the surface boundary of the tetrahedron. We compute the integral over one of the tetrahedrone's surfaces on which makes one triangles of a pentagon because by internal stress equilibrium, those portions cancel with like contributions from the neighboring elements in the assembled force vector of the structure. Hence, the force vector for a tetrahedron takes the form of

$$\mathbf{F}_{3D} = \sum_{i=1}^n \sum_{j=1}^n \mathbf{N}^T \mathbf{t}_{\Delta_1} |\mathbf{J}| w_i w_j \quad (6.112)$$

node	ξ co-ordinate	η co-ordinate	weight
Exact for Polynomials of Degree 1			
1	1/3	1/3	1.0
Exact for Polynomials of Degree 2			
1	2/3	1/6	1/3
2	1/6	1/6	1/3
3	1/6	2/3	1/3
Exact for Polynomials of Degree 3			
1	1/3	1/3	-27/48
2	3/5	1/5	25/48
3	1/5	1/5	25/48
4	1/5	3/5	25/48

Table 6.1: Generalized, Gaussian, weights and nodes for integrating over a triangle in its natural co-ordinate system.

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Appendix A. Implicit Elasticity

Both explicit (Green [102] elastic) and implicit (Rajagopal [103] elastic) material models are put forward in this appendix for one's consideration when choosing a material model to represent biologic fibers and membranes. We discuss thermoelastic fibers first, and then thermoelastic membranes. We have no need to address thermoelastic volumes for our application beyond what has been presented in §4.4.4. We employ Gibbs' free-energy potentials instead of internal-energy potentials to the extent that is possible. They relate to one another via a well-known Legendre transformation. A Gibbs energy approach implies that a change in the intensive variables (thermodynamic forces) will cause a response in the extensive variables (thermodynamic displacements), which is the exact opposite of an internal energy approach. Cause and effect are correct in a Gibbs formulation.

Appendix A.1. Alveolar Chords as Green (Explicit) Thermoelastic Fibers

For a 1D fiber with a mass density of ρ per unit length, the conjugate fields are: temperature θ and entropy η , plus force F and strain $e := \ln(L/L_0)$ with L_0 and L denoting the initial and current fiber lengths. A Green elastic fiber adopts a Gibbs free-energy function with an explicit dependence upon state, viz., $\mathcal{G}(\theta, F)$ such that $d\mathcal{G} = -\eta d\theta - \frac{1}{\rho}e dF$ (cf. Eqn. 4.1a), from which one derives its governing constitutive equations as being

$$\eta = -\partial_\theta \mathcal{G}(\theta, F) \quad \text{and} \quad e = -\rho \partial_F \mathcal{G}(\theta, F) \quad (\text{A.1a})$$

that, when differentiated, can be rearranged into the following hypo-elastic equation

$$\left\{ \begin{array}{l} d\eta \\ de \end{array} \right\} = - \begin{bmatrix} \partial_{\theta\theta} \mathcal{G} & \partial_{\theta F} \mathcal{G} \\ \rho \partial_{F\theta} \mathcal{G} & \rho \partial_{FF} \mathcal{G} \end{bmatrix} \left\{ \begin{array}{l} d\theta \\ dF \end{array} \right\} = \begin{bmatrix} C/\theta & \alpha/\rho \\ \alpha & 1/E \end{bmatrix} \left\{ \begin{array}{l} d\theta \\ dF \end{array} \right\} \quad (\text{A.1b})$$

whose thermo-physical material properties are, in general, functions of state defined by

$$C := \theta \partial_\theta \eta|_F = -\theta \partial_{\theta\theta} \mathcal{G}(\theta, F) \quad (\text{A.1c})$$

$$\alpha := L^{-1} \partial_\theta L|_F = \partial_\theta e|_F = -\rho \partial_{F\theta} \mathcal{G}(\theta, F) \equiv -\rho \partial_{\theta F} \mathcal{G}(\theta, F) \quad (\text{A.1d})$$

$$1/E := L^{-1} \partial_F L|_\theta = \partial_F e|_\theta = -\rho \partial_{FF} \mathcal{G}(\theta, F) \quad (\text{A.1e})$$

where the elastic compliance $1/E = L^{-1} \partial_F L|_\theta = \partial_F \ln(L/L_0)|_\theta = \partial_F e|_\theta$ has units of reciprocal force evaluated at constant temperature, while the thermal expansion coefficient $\alpha = L^{-1} \partial_\theta L|_F = \partial_\theta \ln(L/L_0)|_F = \partial_\theta e|_F$ has units of reciprocal temperature evaluated at constant force. The mass density ρ is one-dimensional in this presentation, i.e., it has units of mass per unit length of fiber; likewise, modulus E has units of force, not stress.

Appendix A.1.1. A Hookean Fiber

A thermoelastic Hookean fiber is Green elastic with a Gibbs free energy described by

$$\mathcal{G}(\theta, F) = -C \left(\theta \ln \left(\frac{\theta}{\theta_0} \right) - (\theta - \theta_0) \right) - \frac{F}{\rho} \left(\alpha(\theta - \theta_0) + \frac{F}{2E} \right) \quad (\text{A.2})$$

which is a function of temperature θ and force F , normalized so that $\mathcal{G}(\theta_0, 0) = 0$, and is compatible with the thermo-physical material properties put forward in Eqn. (A.1c–A.1e). In this model the material constants ρ , C , α and E are all considered to be of constant value across state space.

Appendix A.2. Alveolar Chords as Rajagopal (Implicit) Thermoelastic Fibers

In 2003, Rajagopal [103] introduced the idea of an implicit elastic solid. In 2016, Freed & Rajagopal [90] constructed an elastic fiber model that convolves an explicit energy with an implicit energy. In their approach they decomposed strain $e := \ln(L/L_0)$ into a sum of two strains, viz., $e = e_1 + e_2$ where $e_1 := \ln(L_1/L_0)$ and $e_2 := \ln(L/L_1)$. Length L_0 is an initial fiber length, viz., its length whenever $F = 0$. Length L_1 can be thought of as a fiber length caused solely by an unraveling of molecular configuration (e.g., an unraveling of collagen crimp) under an applied load of F . The state associated with length L_1 is non-physical in that one cannot unravel molecules without also stretching them to some extent. Final length L is the actual fiber length under an applied load F caused by both a reconfiguration and a stretching of its molecular network. Here we present their ideas in terms of a Gibbs free-energy function. (Freed & Rajagopal originally used a Helmholtz free-energy function.)

Let the Gibbs free energy be described by a function of the form¹¹

$$\mathcal{G}(\theta, e, F) := \mathcal{G}_1(e_1, F) + \mathcal{G}_2(\theta, F) \quad \text{where} \quad d\mathcal{G} = -\eta d\theta - \frac{1}{\rho} e dF \quad (\text{A.3})$$

with \mathcal{G}_1 being an implicit potential (a configuration energy) and \mathcal{G}_2 being an explicit potential (a strain energy). This energy function leads to the same constitutive equation displayed in Eqn. (A.1b), but whose material properties (A.1c–A.1e) are now interpreted according to the expressions

$$C := \theta \partial_\theta \eta|_F = -\theta \partial_{\theta\theta} \mathcal{G}_2(\theta, F) \quad (\text{A.4a})$$

$$\alpha := \partial_\theta e|_F = -\rho \partial_{F\theta} \mathcal{G}_2(\theta, F) \equiv -\rho \partial_{\theta F} \mathcal{G}_2(\theta, F) \quad (\text{A.4b})$$

$$1/E := \partial_F e|_\theta = -(\rho \partial_{e_1} \mathcal{G}_1(e_1, F))^{-1} (e + \rho \partial_F \mathcal{G}_2(\theta, e, F)) - \rho \partial_{FF} \mathcal{G}_2(\theta, F) \quad (\text{A.4c})$$

whose elastic compliance $1/E$ is found to be the sum of two compliances: one explicit in origin and the other implicit in origin, and where the mass density ρ is per unit length.

Derivation: Because Gibbs energy is a state function, its differential is exact allowing one to write the left-hand side of the thermodynamic expression $d\mathcal{G} = -\eta d\theta - \frac{1}{\rho} e dF$ as $d\mathcal{G} = \partial_{e_1} \mathcal{G}_1 de_1 + \partial_F \mathcal{G}_1 dF + \partial_\theta \mathcal{G}_2 d\theta + \partial_F \mathcal{G}_2 dF$. Recalling that $e = e_1 + e_2$, the explicit (hyperelastic) terms combine to produce constitutive expressions of

$$\eta = -\partial_\theta \mathcal{G}_2(\theta, F) \quad \text{and} \quad e_2 = -\rho \partial_F \mathcal{G}_2(\theta, F)$$

with the remaining implicit terms collecting to produce the following differential equation

$$\rho \partial_{e_1} \mathcal{G}_1(e_1, F) de_1 = -(e_1 + \rho \partial_F \mathcal{G}_1(e_1, F)) dF.$$

Differentiating the constitutive equation for entropy with respect to state leads directly to the expressions for specific heat C and thermal expansion α stated in Eqns. (A.4a & A.4b).

¹¹One might be tempted to consider an implicit energy function of the form $\mathcal{G} = \mathcal{G}_1(\theta, e_1, F) + \mathcal{G}_2(\theta, F)$, but this would lead to a non-symmetric susceptibility matrix. Consequently, it would not satisfy Maxwell's thermodynamic constraint for integrability; hence, it is inadmissible as a Gibbs potential.

Recalling that the strains add, i.e., $e = e_1 + e_2$, and therefore so do their rates, viz., $de = de_1 + de_2$, a consequence of them being logarithmic in construction, then upon rearranging the implicit constitutive equation to solve for de_1 , while differentiating the explicit constitutive equation for e_2 , and finally adding these strain increments to get de , one obtains the elastic compliance function stated in Eqn. (A.4c). \square

Appendix A.2.1. A Biologic Fiber

The fiber model of Freed & Rajagopal [90] imposes a strain-limiting constraint onto internal strain e_1 whenever one considers a Gibbs free-energy function of the form

$$\mathcal{G}_1(e_1, F) = -\frac{1}{\rho} \left(e_t(E_1 e_1 - F) + 2e_1 F \right) \quad (\text{A.5a})$$

$$\mathcal{G}_2(\theta, F) = -C \left(\theta \ln \left(\frac{\theta}{\theta_0} \right) - (\theta - \theta_0) \right) - \frac{F}{\rho} \left(\alpha(\theta - \theta_0) + \frac{F}{2E_2} \right) \quad (\text{A.5b})$$

which depend upon temperature θ , force F , and internal strain e_1 , normalized so that $\mathcal{G}_1(0, 0) = 0$ and $\mathcal{G}_2(\theta_0, 0) = 0$. In fact, the explicit energy adopted here is Hookean, cf. Eqn. (A.2). The resulting constitutive responses for entropy η and strain $e = \ln(L/L_0)$ are therefore described by the following matrix differential equation

$$\begin{Bmatrix} d\eta \\ de \end{Bmatrix} = \begin{bmatrix} C/\theta & \alpha/\rho \\ \alpha & 1/E \end{bmatrix} \begin{Bmatrix} d\theta \\ dF \end{Bmatrix} \quad (\text{A.5c})$$

with an elastic compliance whose tangent response is described by

$$\frac{1}{E(\theta, e, F)} = \frac{e_t - e_1}{E_1 e_t + 2F} + \frac{1}{E_2} \quad \text{wherein} \quad e_1 = e - \alpha(\theta - \theta_0) - \frac{F}{E_2} \quad (\text{A.5d})$$

with an initial tangent modulus $E(\theta_0, 0, 0)$ of $E_1 E_2 / (E_1 + E_2) \approx E_1$ whenever $E_2 \gg E_1 > 0$, while the terminal tangent modulus $E(e_1 = e_t)$ is E_2 , with a transition strain occurring at $e_t > 0$ that establishes a limiting state for internal strain e_1 , i.e., $0 \leq e_1 < e_t$, which is that strain whereat a fiber's molecular configuration has been completely unraveled. Here ρ is a mass per unit length of fiber, C is a specific heat per unit mass at constant force, and α is a coefficient of linear thermal expansion at constant force, all of which have the same physical interpretation as their counterparts for the Hookean fiber. Only their elastic compliances are interpreted differently. This model has been found to be superior to other models commonly employed in the literature for modeling biologic fibers [104].

Biologic fibers, per our application, are long and slender. Consequently, they will buckle under compression. Buckling is not accounted for in our modeling of alveolar chords. Rather, it is assumed that the compliant response at the origin, with modulus $E_1 E_2 / (E_1 + E_2)$, continues into compression, thereby ensuring a measure of numeric stability in our software.

The above methodology would allow us to construct a suite of thermodynamically admissible elastic compliance functions, but we only have need for the one considered above.

Appendix A.3. Alveolar Septa as Green (Explicit) Thermoelastic Membranes

We observed in §4.2 that an alveolar membrane has a response comprised of an uniform contribution and a non-uniform contribution, and that these two contributions are uncoupled; consequently, their internal energies add in that $\mathcal{U}(\eta, \xi, \varepsilon, \gamma) = \mathcal{U}_u(\eta, \xi) + \mathcal{U}_n(\varepsilon, \gamma)$ with \mathcal{U}_u being the uniform contribution of \mathcal{U} , and \mathcal{U}_n being the non-uniform contribution of \mathcal{U} . It is advantageous to relate the material constants to a Gibbs free-energy approach for the uniform contribution, while retaining the internal energy approach for its non-uniform contribution.

Appendix A.3.1. Uniform Response

From thermodynamics, Eqn. (4.1b), comes $d\mathcal{U}_u = \theta d\eta + \frac{1}{\rho} T dA/A = \theta d\eta + \frac{1}{\rho} \pi d\xi$ where $\pi = 2T$ and $d\xi = \frac{1}{2} A^{-1} dA$ whose mass density ρ now has units of mass per unit area. Upon writing this expression in its Gibbs form $d\mathcal{G}_u = -\eta d\theta - \frac{1}{\rho} \xi d\pi$ via a Legendre transformation comes a constitutive equation appropriate for describing the uniform response of a thermoelastic planar membrane, namely

$$\begin{Bmatrix} d\eta \\ d\xi \end{Bmatrix} = - \begin{bmatrix} \partial_{\theta\theta} \mathcal{G}_u & \partial_{\theta\pi} \mathcal{G}_u \\ \rho \partial_{\pi\theta} \mathcal{G}_u & \rho \partial_{\pi\pi} \mathcal{G}_u \end{bmatrix} \begin{Bmatrix} d\theta \\ d\pi \end{Bmatrix} = \begin{bmatrix} C/\theta & \alpha/2\rho \\ \alpha/2 & 1/4M \end{bmatrix} \begin{Bmatrix} d\theta \\ d\pi \end{Bmatrix} \quad (\text{A.6a})$$

with material constants defined accordingly

$$C := \theta \partial_\theta \eta|_\pi = -\theta \partial_{\theta\theta} \mathcal{G}_u \quad (\text{A.6b})$$

$$\alpha := A^{-1} \partial_\theta A|_T = 2 \partial_\theta \xi|_\pi = -2\rho \partial_{\pi\theta} \mathcal{G}_u = -2\rho \partial_{\theta\pi} \mathcal{G}_u \quad (\text{A.6c})$$

$$1/M := A^{-1} \partial_T A|_\theta = 2 \partial_T \xi|_\theta = 4 \partial_\pi \xi|_\theta = -4\rho \partial_{\pi\pi} \mathcal{G}_u \quad (\text{A.6d})$$

where C is the specific heat at constant pressure, α is the areal coefficient of thermal expansion, and M is the modulus of dilation (uniform expansion). Here η is entropy, θ is temperature, $T := \frac{1}{2}(\sigma_{11} + \sigma_{22})$ is surface tension (an invariant in 2D whose intensive variable is $\pi = 2T = \sigma_{11} + \sigma_{22}$ wherein σ_{ij} are components of Cauchy stress quantified in 2D), and A is area (whose extensive variable is $\xi = \ln \sqrt{A/A_0}$, which denotes dilation, i.e., that strain describing an uniform areal expansion).

Appendix A.3.2. Non-Uniform Response

Because $d\mathcal{U} = d\mathcal{U}_u + d\mathcal{U}_n$ with $d\mathcal{U}_u = \theta d\eta + \frac{1}{\rho} \pi d\xi$ it follows that $d\mathcal{U}_n = \frac{1}{\rho}(\sigma d\varepsilon + \tau d\gamma)$ out of which come constitutive equations that govern the non-uniform response of a Green elastic membrane, viz., $\sigma = \rho \partial_\varepsilon \mathcal{U}_n$ and $\tau = \rho \partial_\gamma \mathcal{U}_n$ which, assuming these are continuous and differentiable functions of state, become the following system of differential equations

$$\begin{Bmatrix} d\sigma \\ d\tau \end{Bmatrix} = \rho \begin{bmatrix} \partial_{\varepsilon\varepsilon} \mathcal{U}_n & \partial_{\varepsilon\gamma} \mathcal{U}_n \\ \partial_{\gamma\varepsilon} \mathcal{U}_n & \partial_{\gamma\gamma} \mathcal{U}_n \end{bmatrix} \begin{Bmatrix} d\varepsilon \\ d\gamma \end{Bmatrix} = \begin{bmatrix} 2N & 2\tau \\ 2\tau & G \end{bmatrix} \begin{Bmatrix} d\varepsilon \\ d\gamma \end{Bmatrix} \quad (\text{A.7a})$$

with material constants defined accordingly

$$N := \Gamma \partial_\Gamma (\mathcal{S}_{11} - \mathcal{S}_{22})|_g = \frac{1}{2} \partial_\varepsilon \pi|_\gamma = \frac{1}{2} \rho \partial_{\varepsilon\varepsilon} \mathcal{U}_n \quad (\text{A.7b})$$

$$G := \Gamma \partial_g \mathcal{S}_{21}|_\Gamma = \partial_\gamma \tau|_\varepsilon = \rho \partial_{\gamma\gamma} \mathcal{U}_n \quad (\text{A.7c})$$

subject to the constraint

$$2\tau = \rho \partial_{\varepsilon\gamma} \mathcal{U}_n = \rho \partial_{\gamma\varepsilon} \mathcal{U}_n \quad (\text{A.7d})$$

which follows from Eqn. (4.15). This constraint suggests that the non-uniform response is actually Rajagopal elastic, because τ is a response variable, with \mathcal{U}_n therefore being an implicit function of state.

Appendix A.3.3. A Hookean Membrane

A Green elastic membrane whose uniform response is governed by a Gibbs free-energy function of the form

$$\mathcal{G}_u(\theta, \pi) = -C \left(\theta \ln \left(\frac{\theta}{\theta_0} \right) - (\theta - \theta_0) \right) - \frac{\pi}{2\rho} \left(\alpha(\theta - \theta_0) + \frac{\pi}{4M} \right) \quad (\text{A.8a})$$

and whose non-uniform response is governed by an internal energy function of the form

$$\mathcal{U}_n(\varepsilon, \gamma) = \mathcal{U}_n(-\varepsilon, \gamma) = \mathcal{U}_n(\varepsilon, -\gamma) = \mathcal{U}_n(-\varepsilon, -\gamma) = \frac{1}{\rho} (2\tau\varepsilon\gamma + N\varepsilon^2 + \frac{1}{2}G\gamma^2) \quad (\text{A.8b})$$

with negative strain arguments accounting for symmetries in strain, which are pertinent for all terms, except for the coupling term $2\tau\varepsilon\gamma$ that arises because of the constraint in Eqn. (A.7d). Form these formulæ come the following system of differential equations

$$\begin{Bmatrix} d\eta \\ d\pi \\ d\sigma \\ d\tau \end{Bmatrix} = \begin{bmatrix} C/\theta - M\alpha^2/\rho & 2M\alpha/\rho & 0 & 0 \\ -2M\alpha & 4M & 0 & 0 \\ 0 & 0 & 2N & 2\tau \\ 0 & 0 & 2\tau & G \end{bmatrix} \begin{Bmatrix} d\theta \\ d\xi \\ d\varepsilon \\ d\gamma \end{Bmatrix} \quad (\text{A.8c})$$

which describes a thermoelastic Hookean membrane whose material parameters ρ , C , α , M , N and G are each constant valued across state space.

Appendix A.4. Alveolar Septa as Rajagopal (Implicit) Thermoelastic Membranes

We employ implicit elasticity here to derive a constitutive theory suitable for describing biologic membranes.

Appendix A.4.1. Biologic Membrane Under Uniform Motions

Like the implicit elastic fiber introduced in Eqn. (A.5), the uniform response of an implicit elastic membrane with a strain-limiting dilation can be modeled using a Gibbs free energy $\mathcal{G}_u(\theta, \xi, \pi) := \mathcal{G}_1(\xi_1, \pi) + \mathcal{G}_2(\theta, \pi)$ where the dilation $\xi := \ln \sqrt{A/A_0}$ is considered to decompose into a sum of two dilations: $\xi_1 := \ln \sqrt{A_1/A_0}$ and $\xi_2 := \ln \sqrt{A/A_1}$ so that $\xi = \xi_1 + \xi_2$, with like interpretations as those from their linear counterparts, viz., e , e_1 and e_2 ; specifically,

$$C := \theta \partial_\theta \eta|_\pi = -\theta \partial_{\theta\theta} \mathcal{G}_2(\theta, \pi) \quad (\text{A.9a})$$

$$\alpha := \partial_\theta \xi|_\pi = -\rho \partial_{\pi\theta} \mathcal{G}_2(\theta, \pi) \equiv -\rho \partial_{\theta\pi} \mathcal{G}_2(\theta, \pi) \quad (\text{A.9b})$$

$$1/M := 4 \partial_\pi \xi|_\theta = -4 \left((\rho \partial_{\xi_1} \mathcal{G}_1(\xi_1, \pi))^{-1} (\xi + \rho \partial_\pi \mathcal{G}_u(\theta, \xi, \pi)) + \rho \partial_{\pi\pi} \mathcal{G}_2(\theta, \pi) \right) \quad (\text{A.9c})$$

whose derivation is analogous to that of the implicit fiber above. In this case, we consider a Gibbs free-energy function of the form

$$\mathcal{G}_1(\xi_1, \pi) = -\frac{1}{\rho} \left(\xi_t (4M_1 \xi_1 - \pi) + 2\xi_1 \pi \right) \quad (\text{A.10a})$$

$$\mathcal{G}_2(\theta, \pi) = -C \left(\theta \ln \left(\frac{\theta}{\theta_0} \right) - (\theta - \theta_0) \right) - \frac{\pi}{2\rho} \left(\alpha(\theta - \theta_0) + \frac{\pi}{4M_2} \right) \quad (\text{A.10b})$$

whose resulting elastic compliance is

$$\frac{1}{M(\theta, \xi, \pi)} = \frac{\xi_t - \xi_1}{M_1 \xi_t + \pi/2} + \frac{1}{M_2} \quad \text{wherein} \quad \xi_1 = \xi - \frac{1}{2}\alpha(\theta - \theta_0) - \frac{\pi}{4M_2} \quad (\text{A.10c})$$

with $\xi_t > 0$ being an upper bound on strain ξ_1 in that $0 \leq \xi_1 < \xi_t$. Such a membrane has an initial tangent stiffness $M(\theta_0, 0, 0)$ of $M_1 M_2 / (M_1 + M_2) \approx M_1$ whenever $M_2 \gg M_1 > 0$, and a terminal tangent stiffness $M(\xi_1 = \xi_t)$ of M_2 .

Membranes will wrinkle under states of negative surface tension (or dilation). In alveolar mechanics, surfactant helps to prevent this, and a possible ensuing alveolar collapse. Wrinkling is not accounted for in our modeling of alveolar septa. Rather, like fibers, membranes are assumed to support compression with a modulus of $M_1 M_2 / (M_1 + M_2)$, which associates with the compliant response found at the origin (zero tension, zero dilation). This is done to help ensure numeric stability in our software.

The difference between a Green and Rajagopal thermoelastic membrane undergoing a dilation is in their definitions for elastic compliance. There is no difference in their properties for specific heat or thermal expansion. The above model has been successfully applied to a visceral pleura membrane [51].

Appendix A.5. Biologic Membrane Under Non-Uniform Motions

We seek an energetic construction that is consistent with that of the Freed & Rajagopal fiber model [90], but which is applicable to the non-uniform responses of planar membranes. A Rajagopal elastic solid is implicit; therefore, we consider an internal energy with the following special structure

$$\mathcal{U}_n(\varepsilon, \gamma, \sigma, \tau) = \frac{1}{\rho} 2\varepsilon\gamma\tau + \mathcal{U}_1(\varepsilon_1, \sigma) + \mathcal{U}_2(\varepsilon_2) + \mathcal{U}_3(\gamma_1, \tau) + \mathcal{U}_4(\gamma_2) \quad (\text{A.11})$$

that depends upon squeeze strains $\varepsilon := \ln \sqrt{\Gamma/\Gamma_0}$, $\varepsilon_1 := \ln \sqrt{\Gamma_1/\Gamma_0}$ and $\varepsilon_2 := \ln \sqrt{\Gamma/\Gamma_1}$, and shear strains $\gamma := g - g_0$, $\gamma_1 := g_1 - g_0$ and $\gamma_2 := g - g_1$, both of which are additive in that $\varepsilon = \varepsilon_1 + \varepsilon_2$ and $\gamma = \gamma_1 + \gamma_2$, and as such, so are their differential rates of change $d\varepsilon = d\varepsilon_1 + d\varepsilon_2$ and $d\gamma = d\gamma_1 + d\gamma_2$. Strains ε_1 and γ_1 may be thought of as describing unravelings of molecular configuration, analogous to e_1 in the fiber model of Eqn. (A.5) and ξ_1 in the uniform membrane model of Eqn. (A.10c). The first term on the right-hand side of Eqn. (A.11) ensures that the constraint in Eqn. (A.7d) is satisfied. Other than this term, no coupling between squeeze and shear is assumed in this energy function. Energies \mathcal{U}_1 and \mathcal{U}_3 are Rajagopal elastic (implicit), while energies \mathcal{U}_2 and \mathcal{U}_4 are Green elastic (explicit).

Given a non-uniform internal energy in the form of Eqn. (A.11), then the squeeze compliance is found to be

$$\frac{1}{N} = 2 \left(\frac{\rho \partial_\sigma \mathcal{U}_1(\varepsilon_1, \sigma)}{\rho \partial_{\varepsilon_2} \mathcal{U}_2(\varepsilon_2) - \rho \partial_{\varepsilon_1} \mathcal{U}_1(\varepsilon_1, \sigma)} + \frac{1}{\rho \partial_{\varepsilon_2 \varepsilon_2} \mathcal{U}_2(\varepsilon_2)} \right) \quad (\text{A.12a})$$

while the shear compliance is found to be

$$\frac{1}{G} = \Gamma \left(\frac{\rho \partial_\tau \mathcal{U}_3(\gamma_1, \tau) + 2\varepsilon\gamma}{\rho \partial_{\gamma_2} \mathcal{U}_4(\gamma_2) - \rho \partial_{\gamma_1} \mathcal{U}_3(\gamma_1, \tau)} + \frac{1 - 2\varepsilon}{\rho \partial_{\gamma_2 \gamma_2} \mathcal{U}_4(\gamma_2)} \right) \quad (\text{A.12b})$$

whose mathematical structure is similar to that of the fiber model presented in Eqn. (A.5). The first terms in the parentheses are Rajagopal elastic. The second terms are Green elastic. The shear compliance $1/G$ has extra terms of $2\varepsilon\gamma$ and $(1 - 2\varepsilon)$ that arise because of the constraint energy $\frac{1}{\rho} 2\varepsilon\gamma\tau$, which is a direct consequence of defining shear as $\tau := \Gamma \mathcal{S}_{21}$. These extra terms are missing in the original, implicit, membrane model derived by Freed *et al.* [51].

Derivation: The First and Second Laws of Thermodynamics, as they pertain to non-uniform contributions of stress power, obey $d\mathcal{U}_n(\varepsilon, \gamma, \sigma, \tau) = \frac{1}{\rho} dW_n$ where, from Eqn. (A.11), one gets $\rho d\mathcal{U}_n = (2\gamma\tau + \rho \partial_{\varepsilon_1} \mathcal{U}_1(\varepsilon_1, \sigma))d\varepsilon_1 + (2\gamma\tau + \rho \partial_{\varepsilon_2} \mathcal{U}_2(\varepsilon_2))d\varepsilon_2 + (\rho \partial_\sigma \mathcal{U}_1(\varepsilon_1, \sigma))d\sigma + (2\varepsilon\tau + \rho \partial_{\gamma_1} \mathcal{U}_3(\gamma_1, \tau))d\gamma_1 + (2\varepsilon\tau + \rho \partial_{\gamma_2} \mathcal{U}_4(\gamma_2))d\gamma_2 + (2\varepsilon\gamma + \rho \partial_\tau \mathcal{U}_3(\gamma_1, \tau))d\tau$ while the right side becomes $dW_n = \sigma d\varepsilon_1 + \sigma d\varepsilon_2 + \tau d\gamma_1 + \tau d\gamma_2$ because of the additivity in strain rates. Gathering like terms result in two Green elastic formulæ that produce the stresses

$$\sigma = 2\gamma\tau + \rho \partial_{\varepsilon_2} \mathcal{U}_2(\varepsilon_2) \quad \text{and} \quad \tau = 2\varepsilon\tau + \rho \partial_{\gamma_2} \mathcal{U}_4(\gamma_2)$$

and two Rajagopal elastic formulæ that govern the internal strains

$$\begin{aligned} \rho \partial_\sigma \mathcal{U}_1(\varepsilon_1, \sigma) d\sigma &= (\pi - 2\gamma\tau - \rho \partial_{\varepsilon_1} \mathcal{U}_1(\varepsilon_1, \sigma))d\varepsilon_1 \\ (2\varepsilon\gamma + \rho \partial_\tau \mathcal{U}_3(\gamma_1, \tau))d\tau &= (\tau(1 - 2\varepsilon) - \rho \partial_{\gamma_1} \mathcal{U}_3(\gamma_1, \tau))d\gamma_1 \end{aligned}$$

that when combined produce the constitutive responses

$$\begin{aligned} \rho \partial_\sigma \mathcal{U}_1(\varepsilon_1, \sigma) d\sigma &= (\rho \partial_{\varepsilon_2} \mathcal{U}_2(\varepsilon_2) - \rho \partial_{\varepsilon_1} \mathcal{U}_1(\varepsilon_1, \sigma))d\varepsilon_1 \\ (2\varepsilon\gamma + \rho \partial_\tau \mathcal{U}_3(\gamma_1, \tau))d\tau &= (\rho \partial_{\gamma_2} \mathcal{U}_4(\gamma_2) - \rho \partial_{\gamma_1} \mathcal{U}_3(\gamma_1, \tau))d\gamma_1. \end{aligned}$$

We now differentiate the Green elastic constitutive equations, thereby putting them into differential form. When doing this, we impose a constraint that the squeeze compliance $1/N$ is to be evaluated at constant shear γ , while the shear compliance $1/G$ is to be evaluated at constant squeeze ε , consequently

$$d\sigma|_\gamma = \rho \partial_{\varepsilon_2 \varepsilon_2} \mathcal{U}_2(\varepsilon_2) d\varepsilon_2 \quad \text{and} \quad d\tau|_\varepsilon = 2\varepsilon d\tau + \rho \partial_{\gamma_2 \gamma_2} \mathcal{U}_4(\gamma_2) d\gamma_2.$$

Because $d\varepsilon = d\varepsilon_1 + d\varepsilon_2$ and $d\gamma = d\gamma_1 + d\gamma_2$, one solves the above equations for strain rate, adds them appropriately, and from these one can thereby construct the two compliances found in Eqn. (A.12) via the expressions

$$\frac{1}{N} = 2 \left. \frac{d\varepsilon}{d\sigma} \right|_\gamma = 2 \left(\left. \frac{d\varepsilon_1}{d\sigma} \right|_\gamma + \left. \frac{d\varepsilon_2}{d\sigma} \right|_\gamma \right) \quad \text{and} \quad \frac{1}{G} = \Gamma \left. \frac{d\gamma}{d\tau} \right|_\varepsilon = \Gamma \left(\left. \frac{d\gamma_1}{d\tau} \right|_\varepsilon + \left. \frac{d\gamma_2}{d\tau} \right|_\varepsilon \right)$$

that when all terms are collected together become Eqn. (A.12). \square

We now seek an energy function (A.11) that produces compliances $1/N$ and $1/G$ with a like mathematical structure to that of Eqn. (A.10c) for dilation, viz., $1/M$; specifically, we shall consider

$$\rho\mathcal{U}_1(\varepsilon_1, \sigma) = \varepsilon_t(N_1\varepsilon_1 - \sigma) + \varepsilon_1\sigma \quad \rho\mathcal{U}_2(\varepsilon_2) = \frac{1}{2}N_2\varepsilon_2^2 \quad (\text{A.13a})$$

$$\rho\mathcal{U}_3(\gamma_1, \tau) = \gamma_t(G_1\gamma_1 - \tau) + \gamma_1\tau \quad \rho\mathcal{U}_4(\gamma_2) = \frac{1}{2}G_2\gamma_2^2 \quad (\text{A.13b})$$

which have the same mathematical structure as the energies for the biologic fiber (A.5) and uniform membrane (A.10). When substituted into Eqn. (A.12), they produce the following thermoelastic compliances

$$\frac{1}{N} = 2 \left(\frac{\varepsilon_t - |\varepsilon_1|}{N_1\varepsilon_t + 2\gamma\tau} + \frac{1}{N_2} \right) \quad \varepsilon_1 = \varepsilon - \frac{\sigma - 2\gamma\tau}{N_2} \quad (\text{A.14a})$$

$$\frac{1}{G} = \Gamma \left(\frac{\gamma_t - 2\varepsilon\gamma - |\gamma_1|}{G_1\gamma_t + 2\varepsilon\tau} + \frac{1 - 2\varepsilon}{G_2} \right) \quad \gamma_1 = \gamma - \frac{(1 - 2\varepsilon)\tau}{G_2} \quad (\text{A.14b})$$

where absolute values are introduced because the squeeze ε and shear γ strains can take on both positive and negative values, viz., they are odd functions, cf. [51]. (Recall that in our construction the material parameters are tangents to response curves—the models are differential.) Like our other biologic models, the squeeze compliance $1/N$ is described by three material parameters: an asymptotic modulus at the reference state of $N_1N_2/(N_1 + N_2) \approx N_1$ whenever $N_2 \gg N_1 > 0$, where N_1 may be thought of as the stiffness of an unstretched molecular network; a terminal modulus N_2 designating a stiffness after this molecular network has been stretched out; and a limiting state of configurational squeeze ε_t . The shear compliance $1/G$ is also described by three material parameters: an asymptotic modulus at the reference state of $G_1G_2/(G_1 + G_2) \approx G_1$ whenever $G_2 \gg G_1 > 0$, a terminal modulus G_2 , and a limiting state of configurational shear γ_t that shifts by $2\varepsilon\gamma$. This shift is a consequence of the stress-strain coupling introduced in shear $\tau := \Gamma S_{21}$.

Appendix B. Overview

These appendices describe interfaces for a software package written in Python whose intent is to model the micro-mechanical response of alveolar sacs that comprise the bulk of the parenchyma in lung tissue. A flow chart for this software is presented in Fig. B.1. The software assumes the following design strategy: *i*) a reference configuration exists (see ¶ below) and three sequential configurations exist that are separated in time by an uniform time step, *ii*) the three sequential configurations associate with steps $n-1$, n and $n+1$, *iii*) co-ordinates for the next configuration are assigned through a vertex's update method (they can be reassigned multiple times at any step along a solution path), *iv*) the advance method relabels the current data to their associated previous data, and then relabels the next data to their associated current data, thereby preparing the data structure of each object within a dodecahedral object for its next step along a solution path, and *v*) the mechanical response is isotropic and can be described by three modes of deformation: dilatation/dilation, squeeze and shear [51, 52].

The initial co-ordinates that locate each vertex in a dodecahedron used to model the alveoli of lung are assigned according to a reference configuration where the pleural pressure (the negative pressure surrounding lung in the pleural cavity) and the transpulmonary pressure (the difference between aleolar and pleural pressures) are both at zero gauge pressure, i.e., *all pressures are atmospheric pressure in the reference state*. This is not a typical physiological state. The pleural pressure is normally negative, sucking the pleural membrane against the wall of the chest. During expiration, the diaphragm is pushed up, reducing the pleural pressure. The pleural pressure remains negative during breathing at rest, but it can become positive during active expiration. The surface tension created by surfactant helps keep most alveoli open during excursions into positive pleural pressures, but not all will remain open. Alveolar recruitment is not addressed here. Under normal conditions, alveoli are their smallest at max expiration. Alveolar size is predominately determined by the transpulmonary pressure. The greater the transpulmonary pressure the greater the alveolar size.

Numerous methods belonging to the classes of these appendices have a string argument that is denoted as `state` which can take on any of the following values:

'c', 'curr', 'current' gets the value for a current configuration

'n', 'next' gets the value for a next configuration

'p', 'prev', 'previous' gets the value for a previous configuration

'r', 'ref', 'reference' gets the value for the reference configuration

Several strings can be used to denote each `state`.

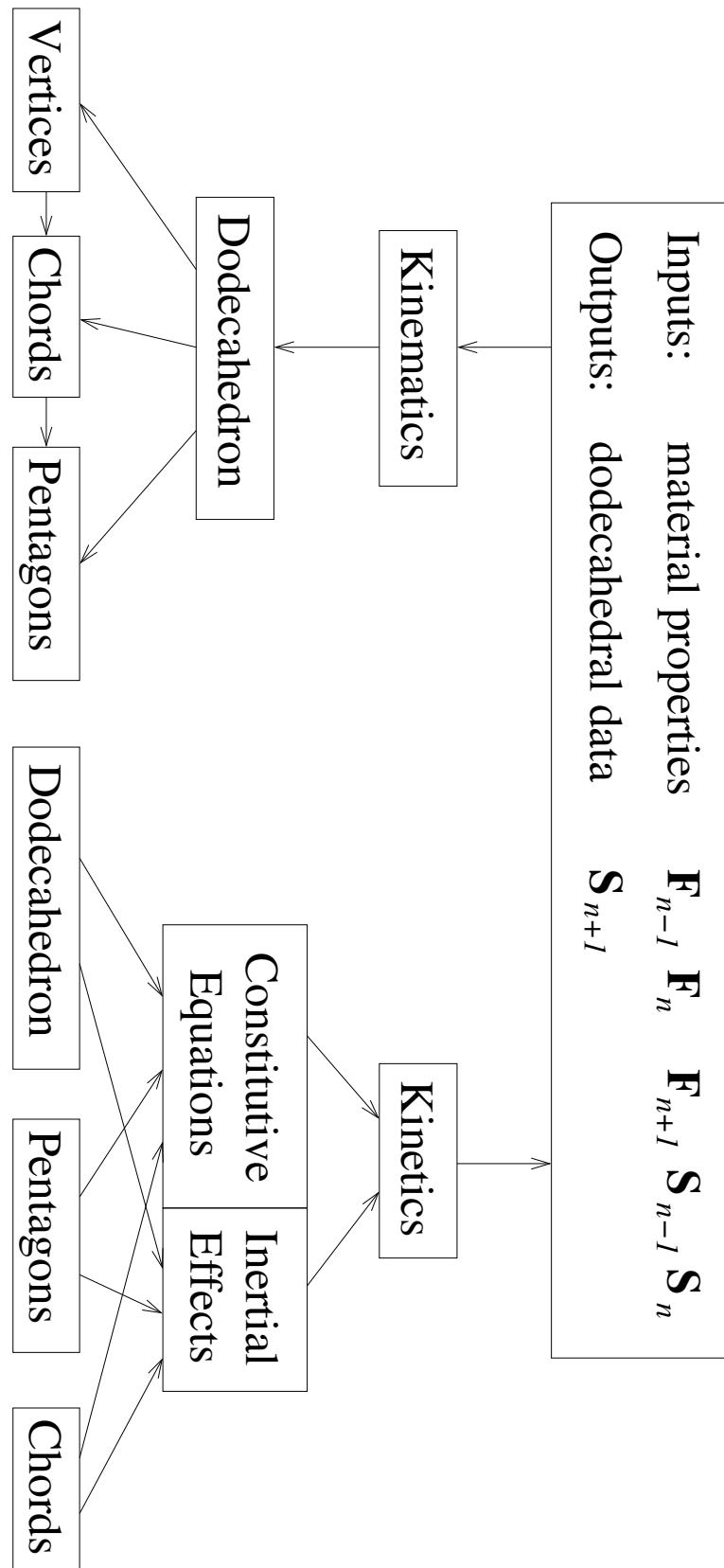


Figure B.1: Flow chart for a dodecahedral model of an alveolus.

Appendix C. Dodecahedra

Module `dodecahedra.py` is Python code that exports class `dodecahedron`. An object of type `dodecahedron` is comprised of twenty vertices labeled according to Table 2.1, as visualized in Fig. 2.1, thirty chords assigned according to Table 2.2, and twelve pentagons assigned according to Table 2.3. This class has the following interface:

`class dodecahedron`

constructor

```
d = dodecahedron(F0, h, gaussPts=1, alveolarDiameter=1.952400802898434)
F0          a deformation gradient: distortion from regular shape in a reference state
h           time step separating two neighboring configurations
gaussPts   number of Gauss points in each pentagonal surface: ∈ {1, 4, 7}
alveolarDiameter mean diameter of an alveolar sac
```

The default alveolar diameter results in vertices of the dodecahedron taking on co-ordinate values that associate with its natural configuration, i.e., all vertices touch the unit sphere from within. Adopting the labeling scheme presented in Fig. 2.1, the vertices are indexed according to Table 2.1, the chords are indexed according to Table 2.2, and the pentagons are indexed according to Table 2.3. If `F0` is the identity matrix, then the shape will be that of a regular dodecahedron in its reference state; otherwise, the shape will be that of an irregular dodecahedron in its reference state. The number of `gaussPts`, viz., 1, 4 or 7, establishes the quadrature scheme to be used for numeric integration, in accordance with Fig. 5.1.

methods

```
s = d.verticesToString(state)
```

Returns a formatted string description for this dodecahedron's vertices in configuration `state`.

```
s = d.chordsToString(state)
```

Returns a formatted string description for this dodecahedron's chords in configuration `state`.

```
s = d.pentagonsToString(state)
```

Returns a formatted string description for this dodecahedron's pentagons in configuration `state`.

```
v = d.getVertex(number)
```

Returns that vertex indexed with `number`, which must be in interval [1, 20].

```
c = d.getChord(number)
```

Returns that chord indexed with `number`, which must be in interval [1, 30].

```
p = d.getPentagon(number)
```

Returns that irregular pentagon indexed with `number`, which must be in interval [1, 12].

```
d.update(nextF)
```

Assuming that the deformation imposed on an alveolus is homogeneous, described by a deformation gradient 'nextF', this procedure assigns new co-ordinate values to all vertices of the dodecahedron for its next configuration such that whenever `nextF` is the identity matrix the dodecahedron is in its reference state. This method calls the `update` methods for all of its vertices, chords and pentagons, after which it updates the local fields of the dodecahedron object itself. This method may be called multiple times before freezing its values with a call to `advance`.

```
d.advance()
```

Calls method `advance` for all of the vertices, chords and pentagons comprising this dodecahedron, where current fields are assigned to previous fields, and then next fields are assigned to current fields for these objects. Afterwards, it assigns the current fields to the previous fields and then assigns the next fields to the current fields of the dodecahedron itself, thereby freezing the present next-fields in preparation for advancing the solution along its path.

The geometric fields associated with a dodecahedron.

```
v = d.volume(state)
```

Returns the volume of this dodecahedron in configuration `state`.

```
vLambda = d.volumetricStretch(state)
```

Returns the cube root of the volume at `state` divided by reference volume, i.e., $\sqrt[3]{V/V_0}$.

```
vStrain = d.volumetricStrain(state)
```

Returns the logarithm of volumetric stretch evaluated at `state`, i.e., $\Xi = \ln \sqrt[3]{V/V_0}$.

```
dvStrain = d.dVolumetricStrain(state)
```

Returns the rate of volumetric strain at `state`, viz., $d\Xi = \frac{1}{3}V^{-1} dV$.

Appendix D. Vertices

Module `vertices.py` is Python code that exports class `vertex`. There are twenty vertices in a dodecahedron. Their normalized reference co-ordinates are presented in Table 2.1, which are indexed according to Fig. 2.1. These normalized co-ordinates are uniformly scaled by the factor `alveolarDiameter/1.952400802898434` supplied to the `dodecahedron` constructor, and then transformed by the linear operator `F0` also supplied to the `dodecahedron` constructor; the vertices are created within the `dodecahedron` constructor. (The user does not call the `vertex` constructor.) This module has the following interface:

function

```
s = coordinatesToString(x, y, z)
  x  the 1 co-ordinate
  y  the 2 co-ordinate
  z  the 3 co-ordinate
```

Returns a formatted string representation for the assigned set of co-ordinates.

`class vertex`

constructor

```
v = vertex(number, x0, y0, z0, h)
  number  an immutable value unique to this vertex
  x0      the initial x co-ordinate at zero pleural pressure
  y0      the initial y co-ordinate at zero pleural pressure
  z0      the initial z co-ordinate at zero pleural pressure
  h       the time-step size between two neighboring configurations
```

co-ordinates `x0`, `y0`, `z0` have values assigned in the reference co-ordinate frame of a dodecahedron. The natural co-ordinates for the vertices of a regular dodecahedron are listed in Table 2.1.

methods

```
s = v.toString(state)
```

Returns a formatted string representation for this vertex in configuration `state` of its dodecahedron.

```
n = v.number()
```

Returns the unique number affiliated with this vertex.

```
x, y, z = v.coordinates(state)
```

Returns the co-ordinates for this vertex in configuration `state`, which are evaluated in the co-ordinate system of its dodecahedron.

```
v.update(x, y, z)
```

Assigns a new set of co-ordinate values to the vertex affiliated with the next configuration of its dodecahedron, as quantified in the co-ordinate system of its dodecahedron. This method may be called multiple times before freezing its value with a call to `advance`. (This method is called internally by `dodecahedron` objects.)

```
v.advance()
```

Assigns all of the object's data associated with the current configuration into their affiliated data associated with the previous configuration, and then assigns all of the object's data associated with the next configuration into their affiliated data associated with the current configuration, thereby freezing these data from external change. (This method is called internally by `dodecahedron` objects.)

Kinematic fields associated with a point (vertex) in 3 space.

```
[ux, uy, uz] = v.displacement(state)
```

Returns the displacement vector of this vertex for configuration `state` whose components are evaluated in the co-ordinate system of its dodecahedron. Displacements interpolate quadratically between consecutive states, because only three locations are maintained at any step n along a solution path.

```
[vx, vy, vz] = v.velocity(state)
```

Returns the velocity vector of this vertex for configuration `state` whose components are evaluated in the co-ordinate system of its dodecahedron. Velocities are calculated using second-order difference formulæ. Velocities interpolate linearly between consecutive states, because only three locations are maintained at any step n along a solution path.

```
[ax, ay, az] = v.acceleration(state)
```

Returns the acceleration vector of this vertex for configuration `state` whose components are evaluated in the co-ordinate system of its dodecahedron. Accelerations are equivalent for the previous, current and next states, i.e., accelerations are constant over an interval $(n-1, n+1)$; consequently, accelerations are discontinuous along a solution path. This is because only three locations are maintained at any step n along a solution path.

Appendix E. Chords

Module `chords.py` is Python code that exports class `chord`. There are thirty chords in a dodecahedron. They are assigned vertices according to Table 2.2 that index according to Fig. 2.1. They are created within the `dodecahedron` constructor. (The user does not call the `chord` constructor.) This class has the following interface:

`class chord`

constructor

`c = chord(number, vertex1, vertex2, h)`

`number` an immutable value unique to this chord

`vertex1` an end point of the chord, an object of class `vertex`

`vertex2` an end point of the chord, an object of class `vertex`

`h` timestep size between two neighboring configurations

Vertices `vertex1` and `vertex2` must be different. The chordal numbering scheme is specified in Table 2.2, given the vertex numbering scheme for the dodecahedron listed in Table 2.1 that is visible in Fig. 2.1.

methods

`s = c.toString(state)`

Returns a formatted string representation for this chord in configuration `state` of its dodecahedron.

`n = c.number()`

Returns the unique number affiliated with this chord.

`v1, v2 = c.vertexNumbers()`

Returns the vertex numbers assigned to the two vertices of this chord.

`truth = c.hasVertex(number)`

Returns `True` if one of the two vertices has this vertex number; otherwise, it returns `False`.

`v = c.getVertex(number)`

Returns the vertex with identifier `number`. Typically, it is to be called inside a `c.hasVertex` `if` clause.

`c.update()`

Establishes the fields that pertain to this instance of `chord` which affiliate with the next configuration. It is to be called after all vertices have had their co-ordinates updated. This method does **not** call the `update` method for the two vertices at its end points. This method may be called multiple times before freezing its values with a call to `advance`. (This method is called internally by `dodecahedron` objects.)

```
c.advance()
```

Assigns all of the object's data associated with the current configuration into their affiliated data associated with the previous configuration, and then assigns all of the object's data associated with the next configuration into their affiliated data associated with the current configuration, thereby freezing these data from external change. This method does **not** call the `advance` method for the two vertices at its end points. (This method is called internally by `dodecahedron` objects.)

The geometric fields associated with a chord in 3 space.

```
ell = c.length(state)
```

Returns the chordal length in configuration `state` of its dodecahedron.

```
lambda = c.stretch(state)
```

Returns the stretch of this chord in configuration `state` of its dodecahedron.

The kinematic fields associated with the centroid of a chord in 3 space.

```
[x, y, z] = c.centroid(state)
```

Returns the position vector for this chord locating its mid-point in configuration `state` of its dodecahedron, i.e., it is the χ vector of Fig. 2.4.

```
[ux, uy, uz] = c.displacement(state)
```

Returns the displacement vector of the centroid for this chord in configuration `state` of its dodecahedron.

```
[vx, vy, vz] = c.velocity(state)
```

Returns the velocity vector of the centroid for this chord in configuration `state` of its dodecahedron.

```
[ax, ay, az] = c.acceleration(state)
```

Returns the acceleration vector of the centroid for this chord in configuration `state` of its dodecahedron.

The rotation and spin matrices for this chord, as measured relative to its dodecahedron's co-ordinate system.

```
pMtx = c.rotation(state)
```

Returns a 3×3 orthogonal matrix \mathbf{P} that rotates the base vectors from its dodecahedral frame of reference into a set of local base vectors where the 1 direction is tangent to the chordal axis, the 2 direction is the normal for this curve in 3 space, and the 3 direction is its binormal. The returned matrix associates with configuration `state` of its dodecahedron.

```
omegaMtx = c.spin(state)
```

Returns a 3×3 skew symmetric matrix $\Omega := \dot{\mathbf{P}}\mathbf{P}^T$ that describes the time rate of rotation, i.e., the spin of the local chordal co-ordinate system about the fixed system of its dodecahedron. The returned matrix associates with configuration `state` of its dodecahedron.

The thermodynamic strain and strain-rate fields associated with a chord.

strain = c.strain(state)

Returns the logarithmic strain for this chord in configuration **state** of its dodecahedron, i.e., $e = \ln(L/L_0)$.

dStrain = c.dStrain(state)

Returns the logarithmic strain-rate for this chord in configuration **state** of its dodecahedron, viz., $de = L^{-1} dL$.

Appendix F. Modules for Planar Pentagons

There are three separate modules that collectively allow a description to be cast for a response of the twelve pentagons that comprise the surface of a dodecahedron. The first module provides their shape functions. The second module provides their kinematics, modeled as membranes. While the third module incorporates these features into a viable description for pentagons.

Appendix F.1. Shape Functions

Module `shapeFunctions` is Python code that exports class `shapeFunction`. These shape functions are for the geometry of an irregular planar pentagon. Shape functions for other geometries are not needed. These objects are created within the `pentagon` constructor, and are utilized by the objects of that class. Class `shapeFunction` has the following interface:

`class shapeFunction`

constructor

`sf = shapeFunction(xi, eta)`

`xi` the x co-ordinate in the natural co-ordinate system

`eta` the y co-ordinate in the natural co-ordinate system

where admissible co-ordinates `xi` and `eta` are any values that lie within the area of that pentagon which inscribes a unit circle or that reside along its boundary, as drawn in Fig. 2.2.

methods

`y = sf.interpolate(y1, y2, y3, y4, y5)`

Returns an interpolation for field `y` at location (`xi, eta`) given values `y1, y2, y3, y4, y5` for some field of interest, which are evaluated at the five vertices of the pentagon, indexed according to Fig. 2.2. Arguments may be of any numeric type or that of a NumPy array.

`Gmtx = sf.G(x1, x2, x3, x4, x5, x01, x02, x03, x04, x05)`

Returns the displacement gradient

$$\mathbf{G} = \begin{bmatrix} \partial u / \partial x & \partial u / \partial y \\ \partial v / \partial x & \partial v / \partial y \end{bmatrix} \quad \text{where} \quad \begin{aligned} u &= x - X \\ v &= y - Y \end{aligned}$$

at that location with natural co-ordinates (`xi, eta`) residing within a pentagonal plane. The arguments are tuples providing co-ordinate positions for the vertices of a pentagon in their pentagonal frame of reference, e.g., `x1 = (x1, y1), ..., x01 = (X1, Y1), ...` with subscripts indexing according to Fig. 2.2.

`Fmtx = sf.F(x1, x2, x3, x4, x5, x01, x02, x03, x04, x05)`

Returns the deformation gradient

$$\mathbf{F} = \begin{bmatrix} \partial x / \partial X & \partial x / \partial Y \\ \partial y / \partial X & \partial y / \partial Y \end{bmatrix}$$

at that location with natural co-ordinates (`xi`, `eta`) residing within a pentagonal plane. The arguments are tuples providing co-ordinate positions for the vertices of a pentagon in their pentagonal frame of reference, e.g., $\mathbf{x1} = (x_1, y_1), \dots, \mathbf{x01} = (X_1, Y_1), \dots$ with subscripts indexing according to Fig. 2.2.

`dFdXi = sf.dFdXi(x1, x2, x3, x4, x5, x01, x02, x03, x04, x05)`

Returns the gradient of a deformation gradient taken with respect to the ξ direction

$$\frac{\partial \mathbf{F}}{\partial \xi} = \frac{\partial}{\partial \xi} \begin{bmatrix} \partial x / \partial X & \partial x / \partial Y \\ \partial y / \partial X & \partial y / \partial Y \end{bmatrix}$$

at that location with natural co-ordinates (`xi`, `eta`) residing within a pentagonal plane. The arguments are tuples providing co-ordinate positions for the vertices of a pentagon in their pentagonal frame of reference, e.g., $\mathbf{x1} = (x_1, y_1), \dots, \mathbf{x01} = (X_1, Y_1), \dots$ with subscripts indexing according to Fig. 2.2.

`dFdEta = sf.dFdEta(x1, x2, x3, x4, x5, x01, x02, x03, x04, x05)`

Returns the gradient of a deformation gradient taken with respect to the η direction

$$\frac{\partial \mathbf{F}}{\partial \eta} = \frac{\partial}{\partial \eta} \begin{bmatrix} \partial x / \partial X & \partial x / \partial Y \\ \partial y / \partial X & \partial y / \partial Y \end{bmatrix}$$

at that location with natural co-ordinates (`xi`, `eta`) residing within a pentagonal plane. The arguments are tuples providing co-ordinate positions for the vertices of a pentagon in their pentagonal frame of reference, e.g., $\mathbf{x1} = (x_1, y_1), \dots, \mathbf{x01} = (X_1, Y_1), \dots$ with subscripts indexing according to Fig. 2.2.

Appendix F.2. Membranes

Module `membranes.py` is Python code that exports class `membrane`. Objects of this class are used to describe kinematic fields at the Gauss points of a pentagon. These objects are created within the `pentagon` constructor, and are utilized by the objects of that class. Class `membrane` has the following interface:

```
class membrane
constructor
m = membrane(h)
    h uniform time step separating any two neighboring configurations
methods
m.update(nextF)
```

Establishes the fields that pertain to this instance of `membrane` which affiliate with the deformation gradient `nextF` of the next configuration. This is a 2×2 matrix describing the deformation gradient in the plane of the pentagon. (It is not the deformation gradient sent to `d.update(nextF)` of `dodecahedron` objects.) This method may be called multiple

times before freezing its values with a call to `advance`. (This method is called internally by `pentagon` objects.)

`m.advance()`

Assigns all of the object's data associated with the current configuration into their affiliated data associated with the previous configuration, and then assigns all of the object's data associated with the next configuration into their affiliated data associated with the current configuration, thereby freezing these data from external change. (This method is called internally by `pentagon` objects.)

Tensor fields that associate with a Gram-Schmidt factorization of the deformation gradient.

`qMtx = m.Q(state)`

Returns the 2×2 re-indexing matrix that is applied to the deformation gradient prior to its Gram-Schmidt decomposition in configuration `state`.

`rMtx = m.R(state)`

Returns the 2×2 rotation matrix **Q** derived from a **QR** decomposition of the re-indexed deformation gradient in configuration `state`.

`omega = m.spin(state)`

Returns the 2×2 spin matrix caused by planar deformation, i.e., $d\mathbf{R}\mathbf{R}^T$, in configuration `state`.

`uMtx = m.U(state)`

Returns the 2×2 Laplace stretch **R** (denoted herein as **U**) derived from a **QR** decomposition of the re-indexed deformation gradient in configuration `state`.

`uInvMtx = m.UIInv(state)`

Returns the 2×2 inverse Laplace stretch **R** (denoted herein as \mathbf{U}^{-1}) derived from a **QR** decomposition of the re-indexed deformation gradient in configuration `state`.

`duMtx = m.dU(state)`

Returns the differential change of the Laplace stretch **R** derived from a **QR** decomposition of the re-indexed deformation gradient in configuration `state`.

`duInvMtx = m.dUIInv(state)`

Returns the differential change of the inverse Laplace stretch **R** derived from a **QR** decomposition of the re-indexed deformation gradient in configuration `state`.

Scalar attributes that arise as extensive thermodynamic variables.

`xi = m.dilation(state)`

Returns the planar dilation derived from a **QR** decomposition of the re-indexed deformation gradient in configuration `state`, i.e., $\xi = \ln \sqrt{A/A_0}$.

```
epsilon = m.squeeze(state)
```

Returns the in-plane squeeze derived from a **QR** decomposition of the re-indexed deformation gradient in configuration `state`, i.e., $\varepsilon = \ln \sqrt{\Gamma/\Gamma_0}$.

```
gamma = m.shear(state)
```

Returns the in-plane shear derived from a **QR** decomposition of the re-indexed deformation gradient in configuration `state`.

```
dXi = m.dDilation(state)
```

Returns a differential change in the planar dilation derived from a **QR** decomposition of the re-indexed deformation gradient in configuration `state`, viz., $d\xi = \frac{1}{2}A^{-1}dA$.

```
dEpsilon = m.dSqueeze(state)
```

Returns a differential change in the planar squeeze derived from a **QR** decomposition of the re-indexed deformation gradient in configuration `state`, viz., $d\varepsilon = \frac{1}{2}\Gamma^{-1}d\Gamma$.

```
dGamma = m.dShear(state)
```

Returns a differential change in the in-plane shear derived from a **QR** decomposition of the re-indexed deformation gradient in configuration `state`.

Appendix F.3. Pentagons

Module `pentagons.py` is Python code that exports class `pentagon`. There are twelve pentagons in a dodecahedron. They are assigned chords according to Table 2.3 with vertices assigned according to Table 2.1 that index according to Fig. 2.1. Pentagon objects are created within the `dodecahedron` constructor. Membrane and shape function objects are created within the `pentagon` constructor. Class `pentagon` has the following interface:

```
class pentagon
```

constructor

```
p = pentagon(number, chord1, chord2, chord3, chord4, chord5, h, gaussPts)
    number      an immutable value unique to this pentagon
    chord1     an edge of the pentagon, an object of class chord
    chord2     an edge of the pentagon, an object of class chord
    chord3     an edge of the pentagon, an object of class chord
    chord4     an edge of the pentagon, an object of class chord
    chord5     an edge of the pentagon, an object of class chord
    h          timestep size between two neighboring configurations
    gaussPts   number of Gauss points in a pentagonal surface: ∈ {1, 4, 7}
```

Chords `chord1`, `chord2`, `chord3`, `chord4`, and `chord5` must have five vertices that are common, assigned according to the scheme presented in Fig. F.2. The pentagon numbering scheme is specified in Table 2.3, given the vertex numbering scheme for the dodecahedron listed in Table 2.1. When assigning the five chords of a pentagon, do so according to

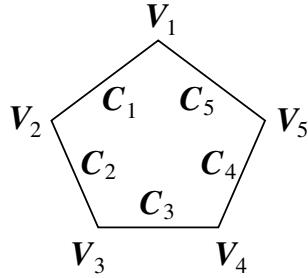


Figure F.2: Vertex and chord labeling scheme for a pentagon, which coincides with the labeling scheme used by the pentagonal shape functions.

Fig. F.2 when looking inward from the outside of a dodecahedron. By numbering the chords in a counterclockwise direction, the algorithm used to compute its area will be positive; otherwise, if the chords were numbered clockwise then the area derived by Eq. (2.12) would become negative.

methods

`s = p.toString(state)`

Returns a formatted string representation for this pentagon in configuration `state`.

`n = p.number()`

Returns the unique number affiliated with this pentagon.

`n1, n2, n3, n4, n5 = p.chordNumbers()`

Returns the chordal numbers associated with the chords of this pentagon, sorted from smallest to largest, i.e., not in accordance to Fig. F.2.

`n1, n2, n3, n4, n5 = p.vertexNumbers()`

Returns the vertex numbers associated with the vertices of this pentagon, sorted from smallest to largest, i.e., not in accordance to Fig. F.2.

`truth = p.hasChord(number)`

Returns `True` if one of the five chords has this chordal number; otherwise, it returns `False`.

`truth = p.hasVertex(number)`

Returns `True` if one of the five vertices has this vertex number; otherwise, it returns `False`.

`c = p.getChord(number)`

Returns the chord with specified `number`. Typically called inside a `p.haschord` `if` clause.

`v = p.getVertex(number)`

Returns the vertex with specified `number`. Typically called inside a `p.hasVertex` `if` clause.

```
v = p.gaussPoints()
```

Returns the number of Gauss points associated with this pentagon.

```
p.update()
```

Establishes the fields that pertain to this object of class `pentagon` that affiliate with the next configuration. It is to be called after all vertices and all chords have been updated. This method does **not** call the `update` methods for the five vertices nor for the five chords that comprise this pentagon, but it does call the `update` methods for the `shapeFunction` and `membrane` objects contained within. This method may be called multiple times before freezing its values with a call to `advance`. (This method is called internally by `dodecahedron` objects.)

```
p.advance()
```

Assigns all of the object's data associated with the current configuration into their affiliated data associated with the previous configuration, and then assigns all of the object's data associated with the next configuration into their affiliated data associated with the current configuration, thereby freezing these data from external change. This method does **not** call the `advance` methods for the five vertices nor for the five chords that make up this pentagon, but it does call the `advance` methods for the `shapeFunction` and `membrane` objects contained within. (This method is called internally by `dodecahedron` objects.)

The geometric fields associated with a pentagonal surface embedded in 3 space.

```
a = p.area(state)
```

Returns the area of this irregular pentagon in configuration `state`.

```
aLambda = p.arealStretch(state)
```

Returns the square root of the area at `state` divided by reference area, i.e., $\sqrt{A/A_0}$.

```
aStrain = p.arealStrain(state)
```

Returns the logarithm of areal stretch evaluated at 'state', i.e., $\ln \sqrt{A/A_0}$.

```
daStrain = p.dArealStrain(state)
```

Returns the rate of areal strain at 'state', viz., $\frac{1}{2}A^{-1} dA$.

```
[nx, ny, nz] = p.normal(state)
```

Returns the outward unit normal vector to this pentagon in configuration `state`.

```
[dnx, dny, dnz] = p.dNormal(state)
```

Returns the rate-of-change of the outward unit normal vector to this pentagon in configuration `state`.

Kinematic vector fields associated with the centroid of a pentagon in 3 space.

```
[cx, cy, cz] = p.centroid(state)
```

Returns the centroid of this irregular pentagon in configuration `state`, i.e., this is vector χ in Fig. 2.5.

```
[ux, uy, uz] = p.displacement(state)
```

Returns the displacement vector of its centroid in configuration `state`.

```
[vx, vy, vz] = p.velocity(state)
```

Returns the velocity vector of its centroid in configuration `state`.

```
[ax, ay, az] = p.acceleration(state)
```

Returns the acceleration vector of its centroid in configuration `state`.

The rotation and spin of a pentagonal surface as it moves through 3 space.

```
pMtx = p.rotation(state)
```

Returns a 3×3 orthogonal matrix \mathbf{P} that rotates the base vectors from its dodecahedral frame of reference into a set of local base vectors pertaining to this irregular pentagon whose outward normal aligns with the 3 direction, i.e., the irregular pentagon resides in the local pentagonal 1-2 plane. The local 1 direction connects the shoulders of the pentagon, while the 2 direction is rooted at the head of the pentagon. The returned matrix associates with configuration `state`.

```
omegaMtx = p.spin(state)
```

Returns a 3×3 skew symmetric matrix $\Omega := d\mathbf{P} \mathbf{P}^T$ that describes the time rate of rotation, i.e., a spin of the local pentagonal co-ordinate system about the fixed co-ordinate system of its dodecahedron. The returned matrix associates with configuration `state`.

The kinematic tensor fields of a planar membrane evaluated in the reference co-ordinate system of the pentagon. To rotate a tensor field from the pentagonal frame, say $\bar{\mathbf{A}}$, into its dodecahedral frame producing \mathbf{A} , apply the following map: $\mathbf{A} = \mathbf{P} \bar{\mathbf{A}} \mathbf{P}^T$ where \mathbf{P} is the orthogonal matrix returned by `rotation`.

```
fMtx = p.F(gaussPt, state)
```

Returns the 2×2 planar deformation gradient \mathbf{F} located at `gaussPt` in configuration `state`.

```
dFdX = p.dFdX(gaussPt, state)
```

Returns the partial derivative taken with respect to the X direction of a 2×2 planar deformation gradient, viz., $\mathbf{F}_{,1}$, located at `gaussPt` in configuration `state`.

```
dFdY = p.dFdY(gaussPt, state)
```

Returns the partial derivative taken with respect to the Y direction of a 2×2 planar deformation gradient, viz., $\mathbf{F}_{,2}$, located at `gaussPt` in configuration `state`.

`gMtx = p.G(gaussPt, state)`

Returns the 2×2 planar displacement gradient **G** located at `gaussPt` in configuration `state`.

`qMtx = p.Q(gaussPt, state)`

Returns the 2×2 re-indexing matrix **Q** located at `gaussPt` in configuration `state`.

`rMtx = p.R(gaussPt, state)`

Returns the 2×2 rotation matrix **R** derived from a **QR** decomposition of the re-indexed deformation gradient, denoted as **RU**, located at `gaussPt` in configuration `state`.

`uMtx = p.U(gaussPt, state)`

Returns the 2×2 Laplace stretch **U** derived from a **QR** decomposition of the re-indexed deformation gradient located at `gaussPt` in configuration `state`.

`uInvMtx = p.UInv(gaussPt, state)`

Returns the inverse of a 2×2 Laplace stretch \mathbf{U}^{-1} derived from a **QR** decomposition of the re-indexed deformation gradient located at `gaussPt` in configuration `state`.

`duMtx = p.dU(gaussPt, state)`

Returns a differential change in the 2×2 Laplace stretch **U** derived from a **QR** decomposition of the re-indexed deformation gradient located at `gaussPt` in configuration `state`.

`duInvMtx = p.dUInv(gaussPt, state)`

Returns a differential change in the inverse of a 2×2 Laplace stretch \mathbf{U}^{-1} derived from a **QR** decomposition of the re-indexed deformation gradient located at `gaussPt` in configuration `state`.

Scalar attributes that are extensive thermodynamic variables, and their rates.

`xi = p.dilation(gaussPt, state)`

Returns the planar dilation derived from a **QR** decomposition of the re-indexed deformation gradient located at `gaussPt` in configuration `state`, i.e., $\xi = \ln \sqrt{ab/a_0 b_0}$.

`epsilon = p.squeeze(gaussPt, state)`

Returns the planar squeeze derived from a **QR** decomposition of the re-indexed deformation gradient located at `gaussPt` in configuration `state`, i.e., $\varepsilon = \ln \sqrt{ab_0/a_0 b}$.

`gamma = p.shear(gaussPt, state)`

Returns the planar shear derived from a **QR** decomposition of the re-indexed deformation gradient located at `gaussPt` in configuration `state`.

`dDelta = p.dDilation(gaussPt, state)`

Returns differential change in the dilation of an irregular pentagon located at `gaussPt` in configuration `state`.

```
dEpsilon = p.dSqueeze(gaussPt, state)
```

Returns differential change in the squeeze of an irregular pentagon located at `gaussPt` in configuration `state`.

```
dGamma = p.dGamma(gaussPt, state)
```

Returns differential change in the shear of an irregular pentagon located at `gaussPt` in configuration `state`.

Appendix G. Constitutive Models

There are elastic constitutive models for 1D fibers, chordal fibers, 2D membranes, and 3D volumes. These are provided for in module `constitutiveEqns.py`.

Appendix G.1. Elastic Fibers

Five constitutive models are considered for 1D elastic fibers. Their mathematical representations are summarized in Eqn. (??). All five inherit the base class `elasticFibers` whose interface is:

```
class elasticFiber
```

implemented methods

These methods are intended to be called via a super call from all classes that extend class `elasticFiber`.

```
<object>.__init__()
```

This is the constructor, but it is not to be called externally, only internally from those classes that extend this base class.

```
name = <object>.fiberType()
```

Returns a string that contains the name of the fiber model.

```
E = <object>.modulus(stress, strain, temperature)
```

Returns the elastic tangent modulus at the specified `stress`, `strain` and `temperature`. It is the inverse of its elastic compliance.

virtual method

This method must be overridden by every fiber model that extends this base type. Virtual methods only provide an interface; their implementation is empty.

```
C = <object>.compliance(stress, strain, temperature)
```

Returns the elastic tangent compliance at the specified `stress`, `strain` and `temperature`.

Appendix G.1.1. Hookean Fibers

This class provides the elastic compliance and modulus for a Hookean fiber per Eqn. (??).

```
class hooke(elasticFiber)
```

constructor

```
elasFiber = hooke(E)
```

`E` the elastic modulus of the fiber, i.e., Young's modulus

```
name = elasFiber.fiberType()
```

Returns a string that contains the name of the fiber model, viz., ‘Hooke’.

```
C = elasFiber.compliance(stress, strain, temperature)
```

Returns the elastic compliance at a specified **stress**, **strain** and **temperature**. None of these arguments are required.

```
E = elasFiber.modulus(stress, strain, temperature)
```

Returns the elastic modulus at a specified **stress**, **strain** and **temperature**, which is the inverse of its elastic compliance. None of these arguments are required.

Appendix G.1.2. Fungean Fibers

This class provides the elastic compliance and modulus for a Fungean fiber per Eqn. (??).

```
class fung1(elasticFiber)
```

constructor

```
elasFiber = fung1(E, beta)
```

E the elastic tangent modulus at zero stress and zero strain

beta strength of the exponential response

```
name = elasFiber.fiberType()
```

Returns a string that contains the name of the fiber model, viz., ‘Fung’.

```
C = elasFiber.compliance(stress, strain, temperature)
```

Returns the elastic tangent compliance at a specified **stress**, **strain** and **temperature**. Only argument **stress** is required.

```
E = elasFiber.modulus(stress, strain, temperature)
```

Returns the elastic tangent modulus at a specified **stress**, **strain** and **temperature**, which is the inverse of its elastic compliance. Only argument **stress** is required.

Appendix G.1.3. Fungean/Hookean Fibers

This class provides the elastic response functions for Fungean and Hookean fibers whose compliances sum, per Eqn. (??).

```
class fung2(elasticFiber)
```

constructor

```
elasFiber = fung2(E1, E2, beta)
```

E1 the elastic tangent modulus at zero stress and zero strain

E2 the elastic tangent modulus at terminal stress

beta strength of the exponential response

```
name = elasFiber.fiberType()
```

Returns a string that contains the name of the fiber model, viz., ‘Fung/Hooke’.

```
C = elasFiber.compliance(stress, strain, temperature)
```

Returns the elastic tangent compliance at a specified **stress**, **strain** and **temperature**. Only argument **stress** is required.

```
E = elasFiber.modulus(stress, strain, temperature)
```

Returns the elastic tangent modulus at a specified **stress**, **strain** and **temperature**, which is the inverse of its elastic compliance. Only argument **stress** is required.

Appendix G.1.4. Freed-Rajagopal Fibers

This class provides the elastic compliance and modulus for a Freed-Rajagopalean fiber per Eqn. (??).

```
class freed1(elasticFiber)
```

constructor

```
elasFiber = freed1(E, e_t)
```

E the elastic tangent modulus at zero stress and zero strain

e_t the limit strain, i.e., the maximum strain allowed

```
name = elasFiber.fiberType()
```

Returns a string that contains the name of the fiber model, viz., ‘Freed-Rajagopal’.

```
C = elasFiber.compliance(stress, strain, temperature)
```

Returns the elastic tangent compliance at a specified **stress**, **strain** and **temperature**. Argument **temperature** is not required, but **stress** and **strain** are.

```
E = elasFiber.modulus(stress, strain, temperature)
```

Returns the elastic tangent modulus at a specified **stress**, **strain** and **temperature**, which is the inverse of its elastic compliance. Argument **temperature** is not required, but **stress** and **strain** are.

Appendix G.1.5. Freed-Rajagopal/Hookean Fibers

This class provides the elastic response functions for Freed-Rajagopalean and Hookean fibers whose compliances sum, per Eqn. (??). This version does not account for thermal straining.

```
class freed2(elasticFiber)
```

constructor

```
elasFiber = freed2(E1, E2, e_t)
```

E1 the elastic tangent modulus at zero stress and strain

E2 the elastic tangent modulus at terminal stress
e_t the limit strain, i.e., the maximum strain allowed

name = elasFiber.fiberType()

Returns a string that contains the name of the fiber model, viz., ‘Freed-Rajagopal/Hooke’.

C = elasFiber.compliance(stress, strain, temperature)

Returns the elastic tangent compliance at a specified **stress** and **strain**. Argument **temperature** is not required, but **stress** and **strain** are.

E = elasFiber.modulus(stress, strain, temperature)

Returns the elastic tangent modulus at a specified **stress** and **strain**; it is the inverse of its elastic compliance. Argument **temperature** is not required, but **stress** and **strain** are.

Appendix G.1.6. Freed-Rajagopal/Kelvin/Hookean Fibers

This class provides the elastic response functions for Freed-Rajagopalean and Kelvin/Hookean fibers whose compliances sum, per Eqn. (??). This version does account for thermal straining.

class freed3(elasticFiber)

constructor

elasFiber = freed3(E1, E2, e_t, alpha, T0)

E1 the elastic tangent modulus at zero stress and strain

E2 the elastic tangent modulus at terminal stress

e_t the limit strain, i.e., the maximum strain allowed

alpha thermal strain coefficient

T0 the reference temperature for thermal strain, typically body temperature

name = elasFiber.fiberType()

Returns a string that contains the name of the fiber model, viz., ‘Freed-Rajagopal/Kelvin/Hooke’.

C = elasFiber.compliance(stress, strain, temperature)

Returns the elastic tangent compliance at a specified **stress**, **strain** and **temperature**. All arguments are required.

E = elasFiber.modulus(stress, strain, temperature)

Returns the elastic tangent modulus at a specified **stress**, **strain** and **temperature**, which is the inverse of its elastic compliance. All arguments are required.

Appendix G.2. Chordal Fibers

Appendix H. Solvers

Two ODE solvers are included in this software. The first, `peceVtoX.py`, uses a two-step PECE (Predict, Evaluate, Correct, re-Evaluate) method to solve a first-order, ordinary differential equation $\dot{\mathbf{x}}(t) = \mathbf{v}(t) = \mathbf{f}(t, \mathbf{x})$ given an initial condition $\mathbf{x}_0 = \mathbf{x}(t_0)$ where, as an analogy, \mathbf{x} denotes displacement and \mathbf{v} denotes velocity. The second, `peceAtoVandX.py`, uses another two-step PECE method to solve a second-order, ordinary, differential equation $\ddot{\mathbf{x}}(t) = \mathbf{a}(t) = \mathbf{f}(t, \mathbf{x}, \mathbf{v})$ given initial conditions $\mathbf{x}_0 = \mathbf{x}(t_0)$ and $\mathbf{v}_0 = \mathbf{v}(t_0) = \dot{\mathbf{x}}(t_0)$ where, as an analogy, \mathbf{x} denotes displacement, \mathbf{v} denotes velocity, and \mathbf{a} denotes acceleration.

Appendix H.1. 1st Order ODE Solver

Module `peceVtoX.py` is a Python code that exports class `pece` which solves first-order, ordinary, differential equations using a two-step method; in particular, it solves

$$\mathbf{v} = \mathbf{f}(t, \mathbf{x}) \quad \text{where} \quad \mathbf{v} = \dot{\mathbf{x}} \quad \text{satisfying IC} \quad \mathbf{x}_0 = \mathbf{x}(t_0)$$

where the dependent variables of integration \mathbf{x} are analogous to displacements, while the ODEs $\dot{\mathbf{x}} = \mathbf{f}(t, \mathbf{x})$ are analogous to velocities $\mathbf{v} = \dot{\mathbf{x}}$.

```
class pece
constructor
solver = pece(ode, t0, x0, h, tol=0.0001)
    ode the differential equation to be solved, i.e.,  $\dot{\mathbf{x}} = \mathbf{v} = \mathbf{f}(t, \mathbf{x})$  where ode =  $\mathbf{f}(t, \mathbf{x})$ 
    t0 the initial time  $t$ , viz., time at the start of integration
    x0 the initial condition, viz., displacements at the start of integration  $\mathbf{x}_0 = \mathbf{x}(t_0)$ 
    h the global time-step size separating two neighboring states
    tol the maximum allowed local truncation error, with a default set at  $10^{-4}$ 
```

methods

`solver.integrate()`

A command that integrates the ODE from current time t_n to the next time $t_{n+1} = t_n + h$. This command may be called multiple times before committing a solution. A local time stepper is used to integrate over the global time step. The local time-step size is controlled by a PI controller that runs in the background. This controller bounds the local truncation error from above. If the error is too small then the controller increases the local step size. If the error is too large then the controller decreases the local step size.

`solver.advance()`

A command that updates the internal data structure of the integrator by relabeling variables assigned to current time t_n to their counterparts associated with previous time t_{n-1} , and then assigning the variables just solved for at time t_{n+1} to their counterparts at time t_n . This performs an incremental advancement of the solution along its trajectory, with $t_n + h$ now becoming the current time.

The following methods are to be called after a solution has been advanced/committed, but before the next integration step is taken.

```
n, nd, nh, nr = solver.getStatistics()
n    total number of local steps taken
nd   total number of local steps taken where the step-size was doubled
nh   total number of local steps taken where the step-size was halved
nr   total number of local steps taken where the integrator was restarted
```

```
t = solver.getT()
```

Returns the current time t , i.e., the independent variable of integration.

```
x = solver.getX()
```

Returns the solution vector \mathbf{x} at current time, i.e., the dependent variables of integration.

```
v = solver.getV()
```

Returns the time rate-of-change in the dependent variables at current time, i.e., the ODEs being solved, their analog being velocities.

```
err = solver.getError()
```

Returns an estimate for the local truncation error err at current time.

```
x = solver.interpolate(atT)
```

Returns the solution $\mathbf{x}(\text{atT})$ at time atT using cubic Hermite interpolation, where atT is located somewhere between the previous t_{n-1} and current t_n times of the integrator.

Appendix H.2. 2nd Order ODE Solver

Module `peceAtoVandX.py` is a Python code that exports class `pece` which solves second-order, ordinary, differential equations using a two-step method; in particular, it solves

$$\mathbf{a} = \mathbf{f}(t, \mathbf{x}, \mathbf{v}) \quad \text{where} \quad \mathbf{a} = \ddot{\mathbf{x}} \quad \text{and} \quad \mathbf{v} = \dot{\mathbf{x}} \quad \text{with ICs} \quad \mathbf{x}_0 = \mathbf{x}(t_0) \quad \text{and} \quad \mathbf{v}_0 = \mathbf{v}(t_0)$$

where the dependent variables of integration \mathbf{x} are analogous to displacements whose rates $\mathbf{v} = \dot{\mathbf{x}}$ are analogous to velocities, while the ODEs $\ddot{\mathbf{x}} = \mathbf{f}(t, \mathbf{x}, \mathbf{v})$ are analogous to accelerations $\mathbf{a} = \dot{\mathbf{v}} = \ddot{\mathbf{x}}$.

This solver is useful when solving dynamics problems, e.g.,

$$\mathbf{M}\mathbf{a} + \mathbf{C}\mathbf{v} + \mathbf{K}\mathbf{x} = \boldsymbol{\phi}(t, \mathbf{x}, \mathbf{v}) \quad \text{or} \quad \mathbf{a} = \mathbf{f}(t, \mathbf{x}, \mathbf{v}) \quad \text{with} \quad \mathbf{f} = \mathbf{M}^{-1}(\boldsymbol{\phi}(t) - \mathbf{C}\mathbf{v} - \mathbf{K}\mathbf{x})$$

where \mathbf{M} is a mass matrix, \mathbf{C} is a damping matrix, \mathbf{K} is a stiffness matrix, and $\boldsymbol{\phi}$ is a forcing function. Typically \mathbf{M} is diagonal so its inverse is trivial.

```

class pece
constructor

solver = pece(aFn, t0, x0, v0, h, tol=0.0001)
aFn the differential equation to be solved, i.e.,  $\ddot{\mathbf{x}} = \mathbf{a} = \mathbf{f}(t, \mathbf{x}, \dot{\mathbf{x}})$  where  $\mathbf{aFn} = \mathbf{f}(t, \mathbf{x}, \mathbf{v})$ 
t0 the initial time  $t$ , viz., time at the start of integration
x0 an initial condition, viz., displacements at the start of integration  $\mathbf{x}_0 = \mathbf{x}(t_0)$ 
v0 an initial condition, viz., velocities at the start of integration  $\mathbf{v}_0 = \mathbf{v}(t_0) = \dot{\mathbf{x}}(t_0)$ 
h the global time-step size separating two neighboring states
tol the maximum allowed local truncation error, with a default set at  $10^{-4}$ 

```

methods

solver.integrate()

A command that integrates the ODE from current time t_n to the next time $t_{n+1} = t_n + h$. This command may be called multiple times before committing a solution. A local time stepper is used to integrate over the global time step. The local time-step size is controlled by a PI controller that runs in the background. This controller bounds the local truncation error from above. If the error is too small then the controller increases the local step size. If the error is too large then the controller decreases the local step size.

solver.advance()

A command that updates the internal data structure of the integrator by relabeling variables assigned to current time t_n to their counterparts associated with previous time t_{n-1} , and then assigning the variables just solved for at time t_{n+1} to their counterparts at time t_n . This performs an incremental advancement of the solution along its trajectory, with $t_n + h$ now becoming the current time.

The following methods are to be called after a solution has been advanced/committed, but before the next integration step is taken.

```

n, nd, nh, nr = solver.getStatistics()
n total number of local steps taken
nd total number of local steps taken where the step-size was doubled
nh total number of local steps taken where the step-size was halved
nr total number of local steps taken where the integrator was restarted

```

t = solver.getT()

Returns the current time **t**, i.e., the independent variable of integration.

x = solver.getX()

Returns the solution vector **x** at current time, i.e., first set of the dependent variables of integration.

```
v = solver.getV()
```

Returns the solution vector `v` at current time, i.e., second set of the dependent variables of integration.

```
a = solver.getA()
```

Returns the time rate-of-change in the velocity variables at current time, i.e., the ODEs being solved, their analog being accelerations.

```
err = solver.getError()
```

Returns an estimate for the local truncation error `err` at current time.

```
x = solver.interpolateX(atT)
```

Returns the solution `x(atT)` at time `atT` using cubic Hermite interpolation, where `atT` is located somewhere between the previous t_{n-1} and current t_n times of the integrator.

```
x = solver.interpolateV(atT)
```

Returns the solution `v(atT)` at time `atT` using cubic Hermite interpolation, where `atT` is located somewhere between the previous t_{n-1} and current t_n times of the integrator.