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Coordinate Indexing Strategies for the Laplace Stretch in Two and Three Dimensions

by Alan D Freed and John D Clayton

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14. ABSTRACT A kinematic framework for finite-strain continuum mechanics invoking an upper triangular factorization of the deformation gradient is advanced. New algorithms for coordinate indexing in two and three dimensions are developed. For a given orthonormal triad, the labeling of axes, which associates Gram rotation with only pure shears, is shown to be the appropriately indexed or pivoted basis in which to construct the Laplace stretch. For transient three-dimensional problems, a single labeling is proposed to enable the greatest agreement with this properly indexed basis over the history of states, which in turn requires advanced knowledge of the deformation path. Results invoking the proposed method are obtained for a lung constitutive model in simulations of dynamic impact. Comparisons with prior results invoking dynamic indexing show that predictions of local injury are less severe when the new method is used with the same constitutive parameters. Although the previous dynamic indexing technique requires no a priori knowledge of deformation (nor is any arbitrary choice of basis required), rapid transients in continuously varying Laplace attributes may arise that accelerate damage kinetics relative to the new, more stable method.					
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1. Introduction

Gram–Schmidt factorization decomposes a square matrix into a product of two factors: an (orthogonal) rotation and a triangular matrix. When the latter is upper triangular, this construction is often referred to as an upper-triangular decomposition or a QR decomposition, where Q and R are a rotation matrix and upper-triangular matrix, respectively.

In the context of continuum mechanics, adopting bold font for tensors, let $\mathbf{F}$ denote the deformation gradient, which is a two-point tensor. Then the Lagrangian form of the triangular decomposition of $\mathbf{F}$ is a direct application^{1,2} of QR factorization. This is herein written as $\mathbf{F} = \mathbf{R}\mathbf{U}$, where the Lagrangian Laplace stretch tensor $\mathbf{U}$ is upper triangular, and generally not simultaneously symmetric (e.g., symmetry would require $\mathbf{U}$ to be diagonal). The Laplace stretch is designated as $\mathbf{U}$ rather than $\mathbf{R}$, since $\mathbf{R}$ is traditionally used to represent a rotation tensor in continuum mechanics literature.³

In the current work, a kinematic framework invoking a QR factorization of the deformation gradient is substantially advanced. Reference, initial, and current configurations of a material body are more precisely distinguished. Various coordinate frames used in analysis of kinematics and subsequently entering constitutive formulations are given particular attention. The analyst’s frame of reference can, but does not always, differ from the observer’s frame as a result of coordinate indexing. New algorithms for coordinate indexing in two and three dimensions are developed. For a given orthonormal triad, the labeling of axes, which associates Gram rotation with only pure shears, is shown to be the appropriate “physical basis” under which to obtain Laplace stretch from QR factorization. This so-called physical basis should not be confused with the Gram-rotated basis, which is also considered to have physical significance with regard to explicit measurements of Laplace stretch components.^{4,5}

For transient three-dimensional (3-D) problems, a uniform “stationary” labeling is proposed to enable the greatest agreement with the physical basis over the history of states, which in turn requires advanced knowledge of the deformation path. If the deformation gradient history is unknown a priori, however, then invariance is broken since the modeler must manually choose (e.g., logically guess) the pivoting matrix and thus the basis for analysis based on knowledge, if it exists, of the expected transient deformation field. For two-dimensional (2-D) problems, a new transient

indexing scheme is also proposed that invokes analytical transformation formulae between the physical frame and observer's frame for Laplace stretch components and their rates. For 3-D problems, such dynamic transformation formulae are not presently available.

The first known works incorporating the QR decomposition of deformation gradient are attributed to McLellan.^{1,2} Contemporary research began with application of the QR decomposition in constitutive models of anisotropic hyperelastic materials.⁶ Compatibility conditions have been analyzed in the context of QR kinematics and differential-geometric concepts.^{7,8} General constitutive frameworks using Lagrangian^{4,5,9} and Eulerian¹⁰ Laplace stretch measures have been forwarded. Advantages of using Laplace stretch, and derivative strain attributes, in constitutive models rather than traditional strain tensors such as the Green strain¹¹ have been described.⁴⁻⁶

A recent body of work¹²⁻¹⁵ has developed and implemented a QR-based constitutive theory for thermomechanics, damage kinetics, and injury prediction in parenchymal tissue of the lung. Numerical simulations invoking the theory in simulations of dynamic blunt impact to the human torso have been reported, including a software manual for implementing the model as a user module in the LS-DYNA code.¹⁶ Related work on lung mechanics has modeled alveolar-scale physics¹⁷ and shock wave decay using a mixture theory.¹⁸

A method for indexing basis vectors for the physical frame of reference was introduced by Freed and Zamani⁴ and described in algorithmic detail by Paul et al.¹⁹ This method is referred to herein as “dynamic indexing” since, in general, the assignment of basis vectors and corresponding pivoting of the deformation gradient from the observer's frame to the physical frame can vary during the time history of deformation. Following McLellan,² the approach taken by Freed, Paul, and co-workers^{4,19} requires that, under the action of Gram rotation $\mathbf{Q}$, the direction aligned with the rotated 1 axis and the direction normal to the rotated 12 plane remain invariant under the Laplace stretch-induced mapping by $\mathbf{U}$.

The indexing methodology to satisfy this requirement, as formalized by Paul et al.,¹⁹ is to select a basis vector from the observer's set of basis vectors whose edge along the selected direction from a representative cube experiences minimal transverse shear. Then a base vector is chosen from those observer's basis vectors whose

12 coordinate plane experiences minimal in-plane shear, with the remaining observer's base vector becoming the third physical basis vector. Paul et al.¹⁹ show that strain attributes of the Laplace stretch tensor are continuous upon invocation of this method of dynamic reindexing, but also remark that components of Gram rotation are discontinuous across a switch of physical basis.

This previous (dynamic) indexing strategy can be recommended without notable adverse consequences when ratios among deformation components are fixed or slowly varying with respect to time. Such is the case for many problems studied previously^{12–15} involving deformation-controlled loading on spatially homogeneous samples of lung tissue. However, more chaotic conditions arise in impact of the torso, as simulated using the dynamic finite element (FE) method,¹⁶ incurring large rotations and finite stretches whose components vary in a non-proportional way.

Projectile penetration and stress wave interactions with surrounding thoracic structures lead to very abrupt changes in individual components of the deformation gradient. When the dynamic pivoting algorithm^{4,19} is activated, such changes can induce a reindexing of the physical basis during the course of the problem, which in turn alters the proportion of pure shear to simple shear components in a sudden, yet still continuous,¹⁹ way. Since the lung constitutive model^{12–14} treats pure shear and simple shear differently, this transient reindexing affects the predicted material response, including stress state and the local damage or injury metric. Rate-dependent aspects are expected to be more significantly affected due to potentially rapid transients in shear strain partitioning. This expectation is confirmed by predictions of rate-dependent lung damage obtained in simulations reported later.

Remaining sections of this work are arranged as follows. Pertinent aspects of continuum mechanics, notably configurations and deformations of a material body, are presented in Section 2. Coordinate systems are introduced in Section 3 for the experimenter (initial), analyst (physical), and Gram-rotated configurations. Indexing methods for 2-D and 3-D deformation paths are defined, with corresponding algorithms presented for pivoting consistent with physical conjecture. Numerical simulations of impact to the human torso, which incorporate a constitutive model for lung tissue that invokes QR kinematics and enable different indexing methods, are described in Section 4. Results obtained from such simulations for different choices of indexing methods, namely the new stationary approach and the prior dynamic

approach, are compared in Section 5. Conclusions are given in Section 6. Appendices A and B contain, respectively, recommended parameters and recent updates to constitutive models for the lung^{12,13} as implemented¹⁶ in the LS-DYNA code.

2. Configurations and Deformations

A body $\mathcal{B}$, in a continuum sense, comprises an infinite set of particles $\{\mathcal{P}\}$ or material points. These particles embed a region in 3-D space $\mathcal{S}$ that associates with an infinite set of places $\{\mathcal{X}\}$ or spatial points. Space $\mathcal{S}$ is taken to be Euclidean to ensure a norm, while body $\mathcal{B}$ is taken to be simply connected to ensure applicability of Stokes' theorem.²⁰ At some current time t_n , each particle $\mathcal{P}$ occupies an unique place $\mathcal{X}_n$ located by a position vector $\mathbf{x}(t_n)$ described with coordinates $x_i(t_n)$, $i = 1, 2, 3$. The set of places $\{\mathcal{X}_n\}$ in space $\mathcal{S}$ that particles $\{\mathcal{P}\}$ of body $\mathcal{B}$ occupy at any given moment t_n in time is referred to as the body's configuration, denoted as κ_n .

Time t is an independent variable in mechanics. In analysis, one often considers a sequence of discrete times $t_0, t_1, \dots, t_N$ where $t_n > t_{n-1} \forall n \in \{1, 2, \dots, N\}$. Time t_0 specifies the initial time of analysis, which is typically set to 0. Time t_n is used to denote a current time somewhere along a solution path that culminates at time t_N . For some of the analyses considered herein, $h := t_n - t_{n-1} \forall n$ designates a uniform step taken in time.

2.1 Reference Configuration

A reference configuration κ_r establishes an embedding of particles $\{\mathcal{P}\}$ into unique places $\{\mathcal{X}_r\}$ where the body $\mathcal{B}$ is considered to be free from strain. Residual stresses are allowed to exist in an elastic body occupying this configuration. A reference configuration need not be physically attainable during a typical deformation history. This is especially true of biologic tissues. A reference configuration also need not be associated with any particular instance in time.

2.2 Initial Configuration

An initial configuration κ_0 establishes an embedding of particles $\{\mathcal{P}\}$ into unique places $\{\mathcal{X}_0\}$ that associate with the beginning of some deformation history of interest. This configuration correlates with time t_0 . Often there is no distinction between κ_r and κ_0 , because deformation analyses very often consider an initial configuration that is strain-free, too. Nevertheless, configurations κ_r and κ_0 may be distinct, in which case the initial configuration is strained, and thus very likely also stressed.

2.3 Current Configuration

A current configuration κ_n establishes an embedding of particles $\{\mathcal{P}\}$ into unique places $\{\mathcal{X}_n\}$ that associate with some current state in a deformation history (i.e., that affiliated with some current time t_n , $n \in \{1, 2, \dots, N\}$). In analysis, one typically advances the current state from, say, time t_{n-1} to time t_n , whose configurations we denote as κ_{n-1} and κ_n , respectively, with κ_n being the present current configuration and κ_{n-1} being the previous current configuration along some solution path of interest.

2.4 Deformation and Deformation Gradient

Deformation is a physical concept represented mathematically by a mapping from one configuration, say κ_0 , into another configuration, say κ_n , that we denote as $\kappa_0 \mapsto \kappa_n$. Deformation is a two-state idea. It does not depend upon the path traversed in going from one configuration to another. It only depends upon two end states. In the above scenario (i.e., $\kappa_0 \mapsto \kappa_n$), such a mapping produces measures for deformation that are relative to configuration κ_0 . If absolute strain is to be the measure of deformation that one seeks, then $\kappa_r \mapsto \kappa_n$ becomes the appropriate deformation mapping to adopt.

Consider a particle $\mathcal{P}$ in body $\mathcal{B}$. Its motion through space, denoted by a vector function $\chi(\mathbf{x}_0, t_n)$, is a homeomorphism that maps points from an initial configuration κ_0 into points belonging to a current configuration κ_n . Because time is fluid, motion χ describes a path along deformation $\kappa_0 \mapsto \kappa_n$ that need not pass through the reference configuration κ_r .

Let the position vectors locating a particle in its initial κ_0 and current κ_n configurations be denoted by $\mathbf{X} := \mathbf{x}_0$ and $\mathbf{x}_n$, respectively, so that $\mathbf{x}_n = \chi(\mathbf{X}, t_n)$. A

deformation gradient $\mathbf{F}_n$ can therefore be defined as

$$\mathbf{F}_n := \partial \chi(\mathbf{X}, t_n) / \partial \mathbf{X} \quad \text{or more simply} \quad \mathbf{F}_n = \partial \mathbf{x}_n / \partial \mathbf{X}, \quad (1)$$

which is a linear transformation that maps a *tangent* vector existing at particle $\mathcal{P}$ of body $\mathcal{B}$ in configuration κ_0 into the set of all tangent vectors belonging to particle $\mathcal{P}$, now located in configuration κ_n . For convenience, we often write $\mathbf{F}$ instead of $\mathbf{F}_n$ whenever such a distinction is superfluous.

The inverse $\mathbf{F}_n^{-1}$ reverses the mapping from configuration κ_n back to configuration κ_0 . In like manner, $\mathbf{F}_n^{-T}$ is a linear transformation that maps a *normal* vector existing at particle $\mathcal{P}$ in configuration κ_0 into the set of all normal vectors belonging to particle $\mathcal{P}$, now located in configuration κ_n , with $\mathbf{F}_n^T$ reversing the mapping of a normal vector from configuration κ_n back to configuration κ_0 .²¹

The Gram–Schmidt process applied to $\mathbf{F}$ in the physical coordinate frame of the analyst, with such frame to be defined explicitly in Section 3, is written as^{4,5}

$$\mathbf{F} = \mathbf{R}\mathbf{U}; \quad \mathbf{R}^{-1} = \mathbf{R}^T, \quad \det \mathbf{R} = 1; \quad \mathbf{U} : \text{upper triangular}. \quad (2)$$

The Laplace stretch tensor is of the following forms in two and three spatial dimensions, respectively:

$$[\mathbf{U}] = \begin{bmatrix} a & a\gamma \\ 0 & b \end{bmatrix} \quad (2\text{-D}); \quad [\mathbf{U}] = \begin{bmatrix} a & a\gamma & a\beta \\ 0 & b & b\alpha \\ 0 & 0 & c \end{bmatrix} \quad (3\text{-D}). \quad (3)$$

Laplace stretch attributes are the set $(a, b, c, \alpha, \beta, \gamma)$. Volume change is measured by $\det \mathbf{F} = abc$, where $c = 1$ in the 2-D case. Components of $\mathbf{U}$ can be computed directly from those of $\mathbf{F}$ without matrix diagonalization or eigenvalue analysis. Closed-form expressions are available elsewhere.^{4–6} Once $\mathbf{U}$ is computed, the Gram rotation can be found via $\mathbf{R} = \mathbf{F}\mathbf{U}^{-1}$, where closed-form expressions likewise exist for components of $\mathbf{U}^{-1}$, which is also upper triangular.^{4,5}

Different notation pervades the mathematics and mechanics literature for the Gram rotation, here written as $\mathbf{R}$, and for the Laplace stretch, here written as $\mathbf{U}$. Notation used here differs from that in our prior work,^{4,5,12} and the present notation parallels that typically used for the polar decomposition of $\mathbf{F}$ into the product of a generally

different rotation matrix and a symmetric, rather than triangular, right stretch tensor.^{3,11} Both the (upper) triangular decomposition and (right) polar decomposition are unique, but the two decompositions generally produce different rotation and stretch tensors. The right-polar decomposition and the upper-triangular decomposition coincide if and only if (iff) $\mathbf{U}$ is diagonal, in which case, $\mathbf{R} = \mathbf{1}$.

3. Coordinate Systems

All coordinate systems are taken to be rectangular Cartesian with orthonormal base vectors. At the foundation of this set of base vectors is a basis $(\mathbf{i}, \mathbf{j}, \mathbf{k})$ fixed in space and time. The basis $(\mathbf{i}, \mathbf{j}, \mathbf{k})$ is user-specified, and it is also referred to as the coordinate frame of the experimentalist or that of the external observer.

In applications discussed in Sections 4 and 5, the user's basis is inherited from a FE model of a human torso.¹⁶ It is from such FE analysis that microscopic boundary conditions are to be extracted for alveolar-level, subscale modeling of soft tissue mechanics and injury. Our microscopic alveolar models experience this deformation history as a homogeneous far-field deformation to which they succumb, per a conjecture established by Freed et al.¹⁷

To ensure an analysis is indifferent to an observer's perspective whenever one adopts the kinematics of Laplace stretch¹⁹—a byproduct of the 1 direction and the 12 plane (whose normal is the 3 direction), both being invariant under mappings of Laplace stretch²—it may become desirable to reindex the inherited coordinate system $(\mathbf{i}, \mathbf{j}, \mathbf{k})$ according to the mapping

$$\left\{ \mathbf{E}_1 \quad \mathbf{E}_2 \quad \mathbf{E}_3 \right\} = \left\{ \mathbf{i} \mathbf{j} \mathbf{k} \right\} \begin{bmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{bmatrix}, \quad (4a)$$

or equivalently

$$\begin{Bmatrix} \mathbf{E}_1 \\ \mathbf{E}_2 \\ \mathbf{E}_3 \end{Bmatrix} = \begin{bmatrix} P_{11} & P_{21} & P_{31} \\ P_{12} & P_{22} & P_{32} \\ P_{13} & P_{23} & P_{33} \end{bmatrix} \begin{Bmatrix} \mathbf{i} \\ \mathbf{j} \\ \mathbf{k} \end{Bmatrix}. \quad (4b)$$

The tensor $\mathbf{P}$ with rectangular components P_{ij} is referred to as the “pivoting matrix.” Notice that $(\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3)$ is the coordinate basis in which, for example, our

parenchymal model is constructed.¹⁷ It is alternatively referred to herein as the “physical basis” or “physical coordinate frame,” though $(\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3)$ should not be confused with the Gram-rotated basis $(\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3)$, which has also been termed a physical basis in prior work.^{4,5} The latter coincides with the former iff $R_{ij} = \delta_{ij}$.

Pivoting matrix $[P_{ij}]$ is obtained by permuting (rearranging) columns of the identity matrix.²² Consequently, matrix $[P_{ij}]$ only relabels coordinate base vectors; it does not rotate them. Specifically, it selects which base vector from set $\{\mathbf{i}, \mathbf{j}, \mathbf{k}\}$ gets labeled as $\mathbf{E}_1$, which one gets labeled as $\mathbf{E}_2$, and which one becomes $\mathbf{E}_3$. The permutation matrix in Eq. 4b is the transpose (and therefore the inverse) of the permutation matrix in Eq. 4a.

Each element of our dodecahedral model,¹⁷ be it a chord or a membrane, has a native coordinate system that rotates out of the user-assigned base vectors $\{\mathbf{i}, \mathbf{j}, \mathbf{k}\}$ according to the following mappings; specifically, base vectors for chords map as

$$\begin{Bmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \mathbf{e}_3 \end{Bmatrix} = \begin{bmatrix} Q_{11} & Q_{21} & Q_{31} \\ Q_{12} & Q_{22} & Q_{32} \\ Q_{13} & Q_{23} & Q_{33} \end{bmatrix} \begin{Bmatrix} \mathbf{i} \\ \mathbf{j} \\ \mathbf{k} \end{Bmatrix}, \quad (5a)$$

while base vectors for membranes map as

$$\begin{Bmatrix} \mathbf{p}_1 \\ \mathbf{p}_2 \\ \mathbf{p}_3 \end{Bmatrix} = \begin{bmatrix} Q_{11} & Q_{21} & Q_{31} \\ Q_{12} & Q_{22} & Q_{32} \\ Q_{13} & Q_{23} & Q_{33} \end{bmatrix} \begin{Bmatrix} \mathbf{i} \\ \mathbf{j} \\ \mathbf{k} \end{Bmatrix}, \quad (5b)$$

where $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ is the coordinate basis of an individual chordal element, while $(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3)$ is the coordinate basis of an individual pentagonal element. Their origins are located at their centroids. Here matrix $[Q_{ij}]$ is a proper orthogonal matrix of rotation. For a chord, $\mathbf{e}_1$ aligns with the direction of the chord, $\mathbf{e}_2$ is its normal, and $\mathbf{e}_3$ is its binormal. For a pentagon, $\mathbf{p}_1$ orients with the direction connecting its shoulders, while $\mathbf{p}_2$ points toward its apex or head, with $\mathbf{p}_3 := \mathbf{p}_1 \times \mathbf{p}_2$ being the outward normal to this plane.

Just as there is a potential need to reindex the coordinate labels in a 3-D analysis to ensure frame indifference via Eq. 4, it may also become necessary to reindex the coordinate directions of the pentagonal coordinate system assigned by Eq. 5b to

ensure a membrane analysis remains indifferent to an observer's choice of frame.¹⁷ This is achieved according to

$$\begin{Bmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \mathbf{e}_3 \end{Bmatrix} = \begin{bmatrix} P_{11} & P_{21} & 0 \\ P_{12} & P_{22} & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} \mathbf{p}_1 \\ \mathbf{p}_2 \\ \mathbf{p}_3 \end{Bmatrix} \quad \text{or} \quad \mathbf{e}_i = P_{ji} \mathbf{p}_j, \quad (6)$$

where permutation matrix $[P_{ij}]$ potentially relabels the three planar base vectors $(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3)$ of a pentagon to ensure frame indifference. Base vectors $\mathbf{e}_3 = \mathbf{p}_3$ align with the outward normal to the pentagonal plane, and as such, one can write the base vectors for a membrane in more condensed expressions of $(\mathbf{e}_1, \mathbf{e}_2)$ and $(\mathbf{p}_1, \mathbf{p}_2)$, with the third direction being known implicitly.

For conformity, base vectors for coordinate systems of alveolar constituents used in our subscale analyses¹⁷ (i.e., chords and pentagons) are denoted collectively as $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$, where it is understood that each constituent, or element, has its own coordinate system.

In terms of the above coordinate transformations, vector and tensor components evaluated in the user's basis $(\mathbf{i}, \mathbf{j}, \mathbf{k})$, for example,

$$\{\mathbf{v}_i\} = \begin{Bmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \\ \mathbf{v}_3 \end{Bmatrix} \quad \text{and} \quad [\mathbf{T}_{ij}] = \begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{bmatrix}, \quad (7a)$$

map into their components evaluated in basis $(\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3)$, viz.,

$$\{v_i\} = \begin{Bmatrix} v_1 \\ v_2 \\ v_3 \end{Bmatrix} \quad \text{and} \quad [T_{ij}] = \begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{bmatrix}, \quad (7b)$$

according to the linear transformations

$$\begin{aligned} \mathbf{v} &= v_i \mathbf{E}_i & \text{where} & \quad v_i = P_{ij} \mathbf{v}_j \\ \mathbf{T} &= T_{ij} \mathbf{E}_i \otimes \mathbf{E}_j & \text{where} & \quad T_{ij} = P_{ik} T_{kl} P_{jl} \end{aligned} \quad (7c)$$

for general 3-D analyses.

Similarly, vector and tensor components map from a user's basis $(\mathbf{i}, \mathbf{j}, \mathbf{k})$ into a chord's basis $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ as

$$\begin{aligned} \mathbf{v} &= v_i \mathbf{e}_i & \text{where } v_i &= Q_{ij} \mathbf{v}_j \\ \mathbf{T} &= T_{ij} \mathbf{e}_i \otimes \mathbf{e}_j & \text{where } T_{ij} &= Q_{ik} \mathbb{T}_{kl} Q_{jl}, \end{aligned} \quad (7d)$$

or into a pentagon's basis $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ as

$$\begin{aligned} \mathbf{v} &= v_i \mathbf{e}_i & \text{where } v_i &= P_{ij} Q_{jk} \mathbf{v}_k \\ \mathbf{T} &= T_{ij} \mathbf{e}_i \otimes \mathbf{e}_j & \text{where } T_{ij} &= P_{ik} Q_{kl} \mathbb{T}_{lm} Q_{nm} P_{jn}, \end{aligned} \quad (7e)$$

wherein repeated subscripts are summed in accordance with Einstein's summation convention.³

There also exist Gram-rotated bases $(\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3)$ that arise naturally during a triangular factorization of the deformation gradient used to construct Laplace stretch.^{4,5} Specifically,

$$\mathbf{g}_i = R_{ji} \mathbf{e}_j \quad \text{in 2-D} \quad (8a)$$

$$\mathbf{g}_i = R_{ji} \mathbf{E}_j \quad \text{in 3-D}, \quad (8b)$$

where the Gram rotation matrix $[R_{ij}]$, like matrix $[Q_{ij}]$, is a proper orthogonal matrix. The physical attributes of Laplace stretch, introduced in Eq. 3, are projections onto these Gram base vectors. The coordinate frame obtained from $(\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3)$ is thus termed a “physical frame” in previous work.^{4,5}

An important but subtle point is *base vectors rotate between two coordinate frames of reference according to the inverse (or transpose) of how vector and tensor components map between these same two coordinate systems*. Figure 1 illustrates this very important yet subtle point. For example, in Fig. 1, the vector components map as

$$\begin{Bmatrix} \bar{x} \\ \bar{y} \end{Bmatrix} = \begin{bmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{bmatrix} \begin{Bmatrix} x \\ y \end{Bmatrix}, \quad (9a)$$

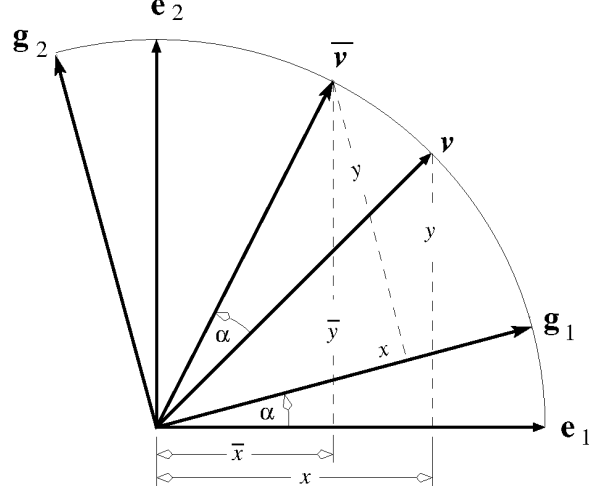


Fig. 1 Rotation of base vectors (e_1, e_2) about axis e_3 into base vectors (g_1, g_2) and of vector $v = xe_1 + ye_2$ into $\bar{v} = \bar{x}e_1 + \bar{y}e_2$

while the coordinate axes map as

$$\begin{Bmatrix} g_1 \\ g_2 \end{Bmatrix} = \begin{bmatrix} \cos \alpha & \sin \alpha \\ -\sin \alpha & \cos \alpha \end{bmatrix} \begin{Bmatrix} e_1 \\ e_2 \end{Bmatrix}, \quad (9b)$$

with base vectors (e_1, e_2) being fixed in space. Throughout this work, orthogonal matrices are assigned components that pertain to how vector and tensor components map between two coordinate frames of reference (cf. Eqs. 4, 5, and 7).

Because all transformation matrices are orthogonal, they obey $P_{ik}P_{jk} = P_{ki}P_{kj} = \delta_{ij}$, $Q_{ik}Q_{jk} = Q_{ki}Q_{kj} = \delta_{ij}$, and $R_{ik}R_{jk} = R_{ki}R_{kj} = \delta_{ij}$, where δ_{ij} is the Kronecker delta (i.e., $\delta_{ij} = 1$ whenever $i = j$, otherwise $\delta_{ij} = 0$), with $\det \mathbf{P} = \pm 1$, $\det \mathbf{Q} = +1$, and $\det \mathbf{R} = +1$. A determinant of $+1$ implies the handedness of a transformed coordinate system is the same as that of the coordinate system out of which it rotated, while a determinant of -1 implies the handedness of the original and final coordinate systems differ. The former class of transformations are rotations, the latter reflections or inversions.

3.1 Coordinates for Laplace Stretch in 2-D

In 2-D analyses, triangular (Laplace) stretch tensors describe a mapping whereby squares deform into parallelograms,⁴ while the more common symmetric (polar) stretch tensors describe a mapping whereby circles deform into ellipses.³ These two measures for stretch have different geometric interpretations that, as a consequence, can affect how their attributes are to be measured in experiments.

Laplace stretch^{1,2,4-6} is a triangular matrix that comes from a Gram–Schmidt factorization, as in Eq. 2, of the deformation gradient $\mathbf{F}$ defined in Eq. 1. It is an upper-triangular matrix in Lagrangian form (a QR factorization in linear algebra) and a lower-triangular matrix in Eulerian form (a LQ factorization in linear algebra).¹⁰ The 2-D and 3-D Lagrangian Laplace stretches, and their associated Gram rotations, are formally introduced in Section 2. Their Eulerian counterparts are not developed for use here, as they lead to more complex constructions not warranted by our application.

In order to use Laplace stretch as one’s primary kinematic field in a membrane analysis, it may become desirable to pivot or reindex the 2-D coordinate system $(\mathbf{p}_1, \mathbf{p}_2)$ assigned to an element via Eq. 5b into a basis that is better suited for analysis,¹⁹ viz., $\mathbf{e}_i = P_{ji}\mathbf{p}_j$ via Eq. 6, such that the components of the deformation gradient obey $\mathbf{F} = \mathcal{F}_{ij}\mathbf{p}_i \otimes \mathbf{p}_j = F_{ij}\mathbf{e}_i \otimes \mathbf{e}_j$, with $\mathcal{F}_{ij} = Q_{ik}F_{kl}Q_{jl}$ and $F_{ij} = P_{ik}\mathcal{F}_{kl}P_{jl}$ in accordance with Eq. 7.

Matrix $[F_{ij}]$, evaluated in a user-supplied coordinate system $(\mathbf{i}, \mathbf{j}, \mathbf{k})$ fixed in space $\mathcal{S}$ and time t , contains the original components of a deformation gradient. In our alveolar application,¹⁷ these components are the prescribed boundary condition. Matrix $[F_{ij}]$, when evaluated in coordinate system $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$, is that matrix upon which Gram–Schmidt factorizations are to be applied.

Whenever one chooses Laplace stretch as one’s foundation for constructing kinematic fields for use in constitutive construction, a reindexing of a 2-D coordinate frame may become desirable because the 1 direction is invariant under transformations of Laplace stretch.² Said differently, Gram rotations ensure that the 1 direction is a physical direction (i.e., that the 1 direction “embeds” within a deforming material⁴). Pivoting, or index relabeling, ensures that this happens in a physically meaningful way.

3.1.1 Dilemma

A need for reindexing, or coordinate relabeling, arises because of a need to manipulate the off-diagonal terms of a deformation gradient (i.e., $\mathcal{F}_{ij}$, $i \neq j$, for membranes) so that the physics of shear does not get misinterpreted due to a possible non-optimal Gram rotation. This procedure assures an indifference to frame (i.e., it provides a systematic means for labeling coordinate axes, independent of user) to ensure that its Gram rotation is physical.

Specifically, for Lagrangian analyses, to the extent that is possible, one seeks to place all, dominant, off-diagonal terms into upper-triangular matrix positions.* Whatever contributions cannot be pivoted into upper-triangular locations will cause a Gram rotation to occur.

3.1.2 Pure Shear

We begin by considering a motion, viz., $\mathbf{x} = \chi(\mathbf{X}, t)$, that describes a planar pure shear, which takes on the form of

$$x_1 = \frac{1}{\sqrt{1 - \gamma^2}} (X_1 + \gamma X_2), \quad (10a)$$

$$x_2 = \frac{1}{\sqrt{1 - \gamma^2}} (\gamma X_1 + X_2), \quad (10b)$$

resulting in a 2×2 deformation gradient with components of

$$[\mathcal{F}_{ij}] = \left[\frac{\partial x_i}{\partial X_j} \right] = \frac{1}{\sqrt{1 - \gamma^2}} \begin{bmatrix} 1 & \gamma \\ \gamma & 1 \end{bmatrix}, \quad (10c)$$

where the coefficient $1/\sqrt{1 - \gamma^2}$ ensures that $\det \mathbf{F} = 1$ (i.e., the area of the plane does not change as a result of this deformation). Geometry requires that $\gamma \in (-1, 1)$ when describing a pure shear, as the spatial dimension would collapse to 1-D if γ were allowed to become ± 1 . There is symmetry between the two off-diagonal terms of a pure shear. This deformation is illustrated in Fig. 2.

The Gram–Schmidt factorization of a planar pure shear produces a deformation

*In an Eulerian analysis, to the extent that is possible, one seeks to place all, dominant, off-diagonal terms into *lower*-triangular matrix positions.

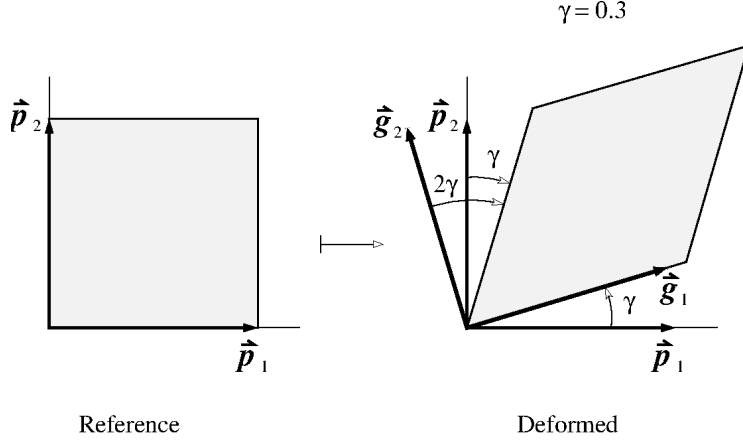


Fig. 2 The pure shear of a unit square deformed into a parallelogram of unit area, where the extent of shear as drawn is $\gamma = 0.3$

gradient with components $F_{ij} = R_{ik}U_{kj}$ * whose Gram rotation matrix is

$$[R_{ij}] = \frac{1}{\sqrt{1+\gamma^2}} \begin{bmatrix} 1 & -\gamma \\ \gamma & 1 \end{bmatrix}, \quad (11a)$$

which results in a coordinate rotation of (see Eq. 8)

$$\begin{Bmatrix} \mathbf{g}_1 \\ \mathbf{g}_2 \end{Bmatrix} = \frac{1}{\sqrt{1+\gamma^2}} \begin{bmatrix} 1 & \gamma \\ -\gamma & 1 \end{bmatrix} \begin{Bmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \end{Bmatrix}. \quad (11b)$$

The matrix of Laplace stretch thereby becomes

$$[U_{ij}] = \frac{1}{\sqrt{1+\gamma^2}\sqrt{1-\gamma^2}} \begin{bmatrix} 1+\gamma^2 & 2\gamma \\ 0 & 1-\gamma^2 \end{bmatrix}, \quad (11c)$$

whose coefficient requires a geometric constraint of $-1 < \gamma < 1$.

*We use the same notation for a Lagrangian decomposition of the deformation gradient that is found in the mechanics literature, viz., $F_{ij} = R_{ik}U_{kj}$. However, here the stretch matrix $[U_{ij}]$ is upper triangular, named after Laplace with matrix $[R_{ij}]$ being its associated Gram rotation with base vectors $\mathbf{g}_i = R_{ji}\mathbf{e}_j$. They arise, collectively, from the Gram–Schmidt factorization of a matrix $[F_{ij}]$ that describes the deformation gradient. Classically, differing from the present work, the stretch matrix $[U_{ij}]$ is symmetric, with matrix $[R_{ij}]$ being its associated rotation. These classic tensors arise from a polar decomposition of the deformation gradient.

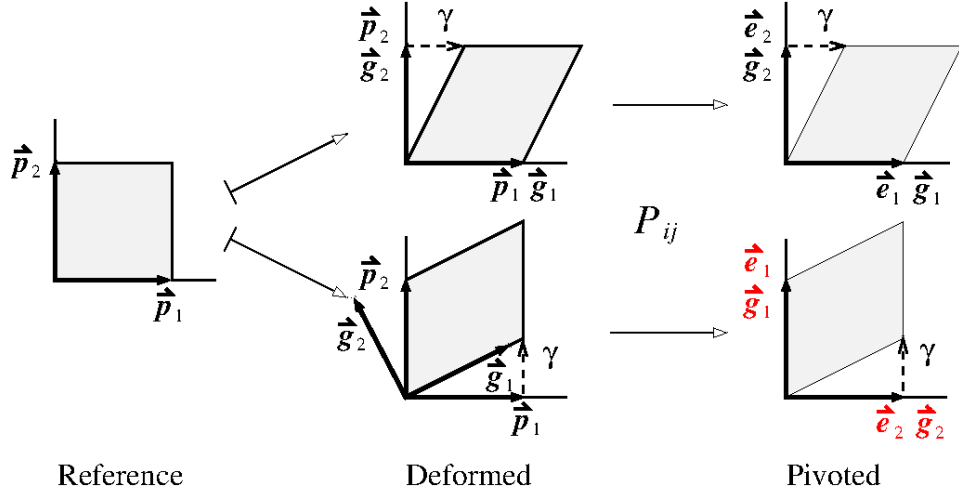


Fig. 3 The left graphic designates a reference configuration. The center graphics designate two deformed configurations: the top a shear in the 1 direction and the bottom a shear in the 2 direction where there is a Gram rotation of basis (g_1, g_2) out of basis (p_1, p_2) . The right graphics designate a mapping of basis (p_1, p_2) into basis (e_1, e_2) through a coordinate permutation P_{ij} , with the relabeled base vectors being shown in red. Pivoting has the effect of there being no Gram rotation of basis (g_1, g_2) out of basis (e_1, e_2) in either case of simple shear. They now provide the same geometric interpretation for simple shear.

The Gram rotation caused by a pure shear is physical, and cannot be avoided. It rotates (e_1, e_2) into (g_1, g_2) , thereby ensuring that g_1 is a material direction⁴ (cf. Fig. 2). For membranes,¹⁷ the Laplace stretch for pure shear comprises two strain attributes: a squeeze (from the diagonal terms) and a shear (from the off-diagonal term).

3.1.3 Simple Shear

Consider the two deformation histories drawn in Fig. 3. Each describes 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. Otherwise, these two deformations are identical. Both shear the 12 plane.

A simple shear in the 1 direction is described by a motion of

$$x_1 = X_1 + \gamma X_2 \quad \text{and} \quad x_2 = X_2, \quad (12a)$$

which results in a deformation gradient with components of

$$[\mathcal{F}_{ij}] = \left[\frac{\partial x_i}{\partial X_j} \right] = \begin{bmatrix} 1 & \gamma \\ 0 & 1 \end{bmatrix}. \quad (12b)$$

A simple shear in the 2 direction is described by a motion of

$$x_1 = X_1 \quad \text{and} \quad x_2 = \gamma X_1 + X_2, \quad (12c)$$

which results in a deformation gradient with components of

$$[\mathcal{F}_{ij}] = \left[\frac{\partial x_i}{\partial X_j} \right] = \begin{bmatrix} 1 & 0 \\ \gamma & 1 \end{bmatrix}. \quad (12d)$$

In both cases, $\det \mathbf{F} = 1$. Consequently, the area of a plane does not change during a simple shearing. The admissible range for a simple shear is without bound, viz., $\gamma \in \mathbb{R}$. Consequently, *the γ of simple shear, where $\gamma \in \mathbb{R}$, is physically different from the γ of pure shear, where $\gamma \in (-1, 1)$.*

The motions of Eq. 12 lead to a Gram–Schmidt factorization of the deformation gradient, viz., $\mathcal{F}_{ij} = R_{ik}U_{kj}$ that, when shear occurs in the 1 direction, is described by

$$[\mathcal{F}_{ij}] = \begin{bmatrix} 1 & \gamma \\ 0 & 1 \end{bmatrix} \implies \begin{cases} [R_{ij}] = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \\ [U_{ij}] = \begin{bmatrix} 1 & \gamma \\ 0 & 1 \end{bmatrix} \end{cases} \quad (13a)$$

but when shear occurs in the 2 direction, is described by

$$[\mathcal{F}_{ij}] = \begin{bmatrix} 1 & 0 \\ \gamma & 1 \end{bmatrix} \Rightarrow \begin{cases} [R_{ij}] = \frac{1}{\sqrt{1+\gamma^2}} \begin{bmatrix} 1 & -\gamma \\ \gamma & 1 \end{bmatrix} \\ [U_{ij}] = \frac{1}{\sqrt{1+\gamma^2}} \begin{bmatrix} 1+\gamma^2 & \gamma \\ 0 & 1 \end{bmatrix} \end{cases} \quad (13b)$$

and as such, two distinct factorizations can result whenever one is describing a planar motion of simple shear. How can this can be? And, how can it be avoided? Answers to these questions follow.

Whenever shear occurs in the 1 direction, its resulting Gram basis $(\mathbf{g}_1, \mathbf{g}_2)$ does not rotate out of $(\mathbf{p}_1, \mathbf{p}_2)$. On the other hand, whenever shear occurs in the 2 direction, its resulting Gram basis $(\mathbf{g}_1, \mathbf{g}_2)$ does rotate out of $(\mathbf{p}_1, \mathbf{p}_2)$. See Fig. 3. This is the cause of our quandary. It is a direct consequence of the 1 direction being invariant under transformations of the Laplace stretch,² and therefore, the 1 direction being a material direction in Laplace kinematics.

In membranes, for the first case of simple shear, the Laplace stretch of Eq. 13a comprises just one strain attribute: a shear (which is correct). However, for the second case of simple shear, the Laplace stretch of Eq. 13b comprises two strain attributes: a squeeze (from the diagonal terms) and a shear (from the off-diagonal term). Yet the considered deformation is just a simple shear.

3.1.4 Remedy

The only difference between the motions that lead to the two deformation gradients presented in Eq. 13 for describing simple shear is in one's choice for labeling the coordinate directions. An unwanted, potential, side effect of this selection process is that, while the Gram rotation in Eq. 13a is physical, the Gram rotation in Eq. 13b is *not* physical. Gram rotations are to be caused by pure shears; they are not to be caused by simple shears. Fortunately, non-physical Gram rotations can be made physical in planar analyses through an appropriate relabeling of the given coordinate axes.

Conjecture 1. *Given an orthonormal coordinate triad, that labeling of its coordinate axes that associates its Gram rotation with pure shears is the appropriate physical rotation to associate with Laplace stretch.*

Matrix operations of row and column pivoting, taken from linear algebra, allow one to transform the lower-triangular form of Eq. 13b into the upper-triangular form of Eq. 13a. This leads to a unified physical interpretation for shearing motions, and it provides a means for establishing a remedy to the above dilemma. Specifically, the extent of shear appearing in the lower-triangular position is a pure shear, while the upper-triangular position holds this pure shear plus a possible contribution caused by simple shear.

For 2-D membranes, two coordinate indexing schemes are possible (for 3-D solids, there are six, to be derived in Section 3.2). The default case is no reindexing of the coordinate axes is required, and as such,

$$[P_{ij}]_1 := \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \implies \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix} := \begin{bmatrix} \mathcal{F}_{11} & \mathcal{F}_{12} \\ \mathcal{F}_{21} & \mathcal{F}_{22} \end{bmatrix}. \quad (14a)$$

In the second case, there is a reindexing specified by

$$[P_{ij}]_2 := \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \implies \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix} := \begin{bmatrix} \mathcal{F}_{22} & \mathcal{F}_{21} \\ \mathcal{F}_{12} & \mathcal{F}_{11} \end{bmatrix}, \quad (14b)$$

where components $F_{ij} = P_{ik}\mathcal{F}_{kl}P_{jl}$ are the ones to be used in Gram–Schmidt factorization, with permutation $\mathbf{P} \in \{\mathbf{P}_1, \mathbf{P}_2\}$ being orthogonal (i.e., $P_{ik}P_{jk} = P_{ki}P_{kj} = \delta_{ij}$ with $\det \mathbf{P} = \pm 1$), specifically, $\det \mathbf{P}_1 = +1$ while $\det \mathbf{P}_2 = -1$. These components associate with $\mathbf{F} = F_{ij}\mathbf{e}_i \otimes \mathbf{e}_j = \mathcal{F}_{ij}\mathbf{p}_i \otimes \mathbf{p}_j$, where $\mathbf{e}_i = P_{ji}\mathbf{p}_j$.

The challenge is in properly selecting $\mathbf{P}_1$ (Case 1) vs. $\mathbf{P}_2$ (Case 2). To this end, it is useful to consider the general motion $\mathbf{x} = \chi(\mathbf{X}, t)$ of a planar membrane illustrated in Fig. 4, specifically,

$$x_1 = xX_1 + \gamma_u yX_2, \quad (15a)$$

$$x_2 = \gamma_l xX_1 + yX_2, \quad (15b)$$

which results in a deformation gradient with components of

$$[\mathcal{F}_{ij}] = \left[\frac{\partial x_i}{\partial X_j} \right] = \begin{bmatrix} x & \gamma_u y \\ \gamma_l x & y \end{bmatrix}, \quad (15c)$$

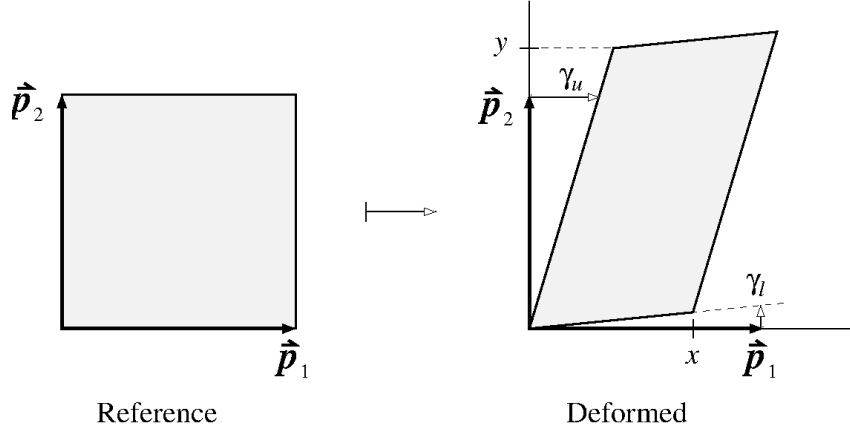


Fig. 4 The general deformation of a unit square into a parallelogram, per Eq. 15, where for example, $x = 0.7$, $y = 1.2$, $\gamma_u = 0.3$, and $\gamma_l = 0.1$, as measured in the $(\mathbf{p}_1, \mathbf{p}_2)$ orthonormal coordinate frame

wherein $x := \mathcal{F}_{11}$ and $y := \mathcal{F}_{22}$ are elongations, while the ratios $\gamma_u := \mathcal{F}_{12}/\mathcal{F}_{22}$ and $\gamma_l := \mathcal{F}_{21}/\mathcal{F}_{11}$ are magnitudes of shear, all evaluated in the $(\mathbf{p}_1, \mathbf{p}_2)$ coordinate frame.

Note that the determinant of deformation gradient is invariant with respect to pivoting and should be positive to ensure positive volume in 3-D analysis^{3,20}: $\det \mathbf{F} = \det[\mathbf{F}_{ij}] = \det[\mathcal{F}_{ij}] > 0$. Physics requires $\gamma_u \gamma_l < 1$, because $\det \mathbf{F} = xy(1 - \gamma_u \gamma_l) > 0$. This geometric constraint (i.e., $\det \mathbf{F} > 0$) is necessary to ensure that the dimension of 2 space does not collapse to unity, another way of saying that area, the analog of volume in 2-D situations, remains positive.

Conjecture 1 provides a strategy for uniquely selecting one of two permutation matrices $\mathbf{P}_1$ and $\mathbf{P}_2$ listed in Eq. 14. This strategy is implemented in Algorithm 1.

input : A deformation gradient matrix $[\mathcal{F}_{ij}]$ evaluated in $(\mathbf{p}_1, \mathbf{p}_2)$, meaning in the membrane's coordinates.

output: A deformation gradient matrix $[F_{ij}]$ evaluated in $(\mathbf{e}_1, \mathbf{e}_2)$, per the permutation matrix $[P_{ij}]$.

if $|\gamma_u| \geq |\gamma_l|$ **then**

 | Case 1: $(\mathbf{p}_1, \mathbf{p}_2) \mapsto (\mathbf{e}_1, \mathbf{e}_2)$, use Eq. 14a

else

 | Case 2: $(\mathbf{p}_2, \mathbf{p}_1) \mapsto (\mathbf{e}_1, \mathbf{e}_2)$, use Eq. 14b

Algorithm 1: Possible reindexing of a 2-D coordinate system to ensure an optimal Laplace stretch. Selected matrices $[P_{ij}]$ and $[F_{ij}]$ are listed in Eq. 14.

In terms of the deformation gradient put forward in Eq. 15, the two axis-labeling cases of Eqs. 14a and 14b can be expressed as

$$\begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix} = \begin{cases} \text{Case 1 :} & \begin{bmatrix} x & \gamma_u y \\ \gamma_l x & y \end{bmatrix} = \begin{bmatrix} \mathcal{F}_{11} & \mathcal{F}_{12} \\ \mathcal{F}_{21} & \mathcal{F}_{22} \end{bmatrix} \\ \text{Case 2 :} & \begin{bmatrix} y & \gamma_l x \\ \gamma_u y & x \end{bmatrix} = \begin{bmatrix} \mathcal{F}_{22} & \mathcal{F}_{21} \\ \mathcal{F}_{12} & \mathcal{F}_{11} \end{bmatrix} \end{cases} \quad (16a)$$

where $F_{ij} = P_{ik} \mathcal{F}_{kl} P_{lj}$ provides the matrix $[F_{ij}]$ to which Gram–Schmidt factorization is to be applied. The Gram rotations that associate with these two indexing cases are given by

$$[R_{ij}] = \begin{cases} \text{Case 1 } (|\gamma_u| \geq |\gamma_l|) : & \frac{1}{\sqrt{1+\gamma_l^2}} \begin{bmatrix} 1 & -\gamma_l \\ \gamma_l & 1 \end{bmatrix} \\ \text{Case 2 } (|\gamma_l| \geq |\gamma_u|) : & \frac{1}{\sqrt{1+\gamma_u^2}} \begin{bmatrix} 1 & -\gamma_u \\ \gamma_u & 1 \end{bmatrix} \end{cases} \quad (16b)$$

which are pure-shear rotations per Eq. 11. Consequently, the Laplace stretches that follow from Algorithm 1 are given by

$$[U_{ij}] = \begin{cases} \text{Case 1 : } \frac{1}{\sqrt{1+\gamma_l^2}} \begin{bmatrix} x(1+\gamma_l^2) & y(\gamma_u+\gamma_l) \\ 0 & y(1-\gamma_u\gamma_l) \end{bmatrix} \\ \text{Case 2 : } \frac{1}{\sqrt{1+\gamma_u^2}} \begin{bmatrix} y(1+\gamma_u^2) & x(\gamma_u+\gamma_l) \\ 0 & x(1-\gamma_u\gamma_l) \end{bmatrix} \end{cases}. \quad (16c)$$

In accordance with Conjecture 1, Algorithm 1 selects the smaller of $|\gamma_u|$ and $|\gamma_l|$ to associate with a pure shear, leaving the larger contribution to associate with both pure and simple shears.

3.1.5 Discontinuity of 2-D Laplace Stretch Attributes

The two cases can switch whenever $|\gamma_u| = |\gamma_l|$, so there is continuity in the Gram rotation across such a switch, as is clear from Eq. 16b, but not necessarily so for the attributes of Laplace stretch evident from Eq. 16c. As mentioned in Section 1, we have also considered elsewhere a dynamic switching strategy where continuity exists in the Laplace attributes, but not for the Gram rotations.¹⁹ Ideally, switching between cases should occur dynamically, independent of user influence, while traversing a path of deformation, thereby instilling a quality of frame indifferent into the kinematics.

For membranes, the 2-D Laplace stretch is described in terms of three stretch attributes, specifically,

$$[U_{ij}] = \begin{cases} \text{Case 1 : } \begin{bmatrix} a & a\gamma \\ 0 & b \end{bmatrix} \\ \text{Case 2 : } \begin{bmatrix} \bar{a} & \bar{a}\bar{\gamma} \\ 0 & \bar{b} \end{bmatrix} \end{cases} \quad (17a)$$

whose time rates of change give rise to a stretch rate (i.e., differentials) of

$$[dU_{ij}] = \begin{cases} \text{Case 1 :} & \begin{bmatrix} da & \gamma da + a d\gamma \\ 0 & db \end{bmatrix} \\ \text{Case 2 :} & \begin{bmatrix} d\bar{a} & \bar{\gamma} d\bar{a} + \bar{a} d\bar{\gamma} \\ 0 & d\bar{b} \end{bmatrix} \end{cases}. \quad (17b)$$

Scalars a and b are elongations, while γ is the extent of shear in the user's frame of reference (i.e., Case 1), with da , db , and $d\gamma$ denoting their rates (e.g., $da = \dot{a} dt$). Likewise, $\bar{a}$ and $\bar{b}$ are elongations, while $\bar{\gamma}$ is the extent of shear whenever Case 2 applies, with $d\bar{a}$, $d\bar{b}$, and $d\bar{\gamma}$ denoting their rates.

Whenever membrane constitutive equations are constructed in a coordinate frame assigned by the user (i.e., here the observer's or experimentalist's local frame $(\mathbf{p}_1, \mathbf{p}_2)$ for an individual [pentagonal] 2-D membrane element), the stretch attributes of Case 2 must be scaled to those of Case 1 (the user's case) for implementation in constitutive equations. The stretch attributes for both cases are given by

$$a = x \frac{1 + \gamma_l^2}{\sqrt{1 + \gamma_l^2}} \quad \bar{a} = y \frac{1 + \gamma_u^2}{\sqrt{1 + \gamma_u^2}} \quad (18a)$$

$$b = y \frac{1 - \gamma_u \gamma_l}{\sqrt{1 + \gamma_l^2}} \quad \bar{b} = x \frac{1 - \gamma_u \gamma_l}{\sqrt{1 + \gamma_u^2}} \quad (18b)$$

$$\gamma = \frac{y \gamma_u + \gamma_l}{x \sqrt{1 + \gamma_l^2}} \quad \bar{\gamma} = \frac{x \gamma_u + \gamma_l}{y \sqrt{1 + \gamma_u^2}}. \quad (18c)$$

To enforce continuity between these stretch attributes and their rates across such a switch, the following maps are then derived:

$$a = \frac{x}{y} \bar{a} \quad da = \frac{x}{y} d\bar{a} + a \frac{dx}{x} - \bar{a} \frac{dy}{y} \quad (18d)$$

$$b = \frac{y}{x} \bar{b} \quad db = \frac{y}{x} d\bar{b} + b \frac{dy}{y} - \bar{b} \frac{dx}{x} \quad (18e)$$

$$\gamma = \left(\frac{y}{x}\right)^2 \bar{\gamma} \quad d\gamma = \left(\frac{y}{x}\right)^2 d\bar{\gamma} + \gamma \frac{d(y/x)}{y/x} - \bar{\gamma} \frac{d(x/y)}{x/y}. \quad (18f)$$

Equations 18d–18f describe the attributes a , b , and γ , and their rates da , db , and $d\gamma$, of Case 1 as scaled quantities of the attributes $\bar{a}$, $\bar{b}$, and $\bar{\gamma}$, and their rates $d\bar{a}$, $d\bar{b}$, and $d\bar{\gamma}$, of Case 2, whenever Case 2 is active. These scalings depend upon the

elongations, but not upon the shears.

Equation 18 establishes the stretch attributes in an experimentalist's frame $(\mathbf{p}_1, \mathbf{p}_2)$ in which constitutive equations can be written, viz., those of Case 1, whenever the Gram–Schmidt process is to be applied to the pivoted Case 2. Consequently, according to these procedures, the selection of Case 1 over Case 2, or vice versa, can be made on the fly, independent of the coordinate labeling scheme selected by the user when they cast their problem for analysis. This transient indexing procedure would not, however, necessarily produce the same results were constitutive equations to be written in terms of Laplace stretch attributes obtained from triangular factorization in the physical frame $(\mathbf{e}_1, \mathbf{e}_2)$.

3.2 Coordinates for Laplace Stretch in 3-D

In 3-D analyses, triangular (Laplace) stretch tensors describe a mapping whereby cubes deform into parallelepipeds,⁴ while the more common symmetric (classic) stretch tensors describe a mapping whereby spheres deform into ellipsoids.³ Therefore, these two measures for stretch have different geometric interpretations that, as a consequence, potentially affect how their attributes can be measured in experiments.

To be able to use Laplace stretch as one's primary kinematic field, as with membranes, it may become desirable to pivot or reindex the 3-D coordinate system $(\mathbf{i}, \mathbf{j}, \mathbf{k})$ inherited from the external observer into a physical basis $(\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3)$ that is “optimally” suited for analysis. By optimal we mean that the ensuing extent of Gram rotation is minimized over a deformation history.

McLellan² proved that the 1 coordinate direction and the normal to the 12 coordinate plane, viz., the 3 coordinate direction, remain invariant under transformations of Laplace stretch over a deformation history. With this fact in mind, we consider a reindexing scheme that minimizes the extent of Gram rotation. Such a Gram rotation is caused by the pure shear contributions to a deformation gradient, in accordance with Conjecture 1. Algorithm 2 selects the appropriate case to apply.

input : A deformation gradient matrix $[F_{ij}]$ evaluated in (i, j, k) , per the user.

output: A deformation gradient matrix $[F_{ij}]$ evaluated in (E_1, E_2, E_3) , per the permutation matrix $[P_{ij}]$.

```

if  $|\gamma_u| \geq |\gamma_l|$  then
  if  $|\alpha_u| \geq |\alpha_l|$  then
    | Case 1:  $(i, j, k) \mapsto (E_1, E_2, E_3)$ , cf. Eq. 20a
  else if  $|\beta_u| \geq |\beta_l|$  then
    | Case 2:  $(i, k, j) \mapsto (E_1, E_2, E_3)$ , cf. Eq. 20b
  else
    | Case 5:  $(k, i, j) \mapsto (E_1, E_2, E_3)$ , cf. Eq. 20e
else
  if  $|\alpha_l| \geq |\alpha_u|$  then
    | Case 6:  $(k, j, i) \mapsto (E_1, E_2, E_3)$ , cf. Eq. 20f
  else if  $|\beta_l| \geq |\beta_u|$  then
    | Case 3:  $(j, k, i) \mapsto (E_1, E_2, E_3)$ , cf. Eq. 20c
  else
    | Case 4:  $(j, i, k) \mapsto (E_1, E_2, E_3)$ , cf. Eq. 20d

```

Algorithm 2: Potential reindexing of the coordinate system to ensure an optimal Laplace stretch. Selected matrices $[P_{ij}]$ and $[F_{ij}]$ are listed in Eq. 20.

Generalizing the strategy developed for 2-D membranes to three dimensions, components of the deformation gradient $\mathbf{F}$ of Eq. 1 in the observer's frame of reference with basis (i, j, k) can be expressed as follows in 3×3 matrix form:

$$[F_{ij}] = \begin{bmatrix} \lambda_x & \gamma_u \lambda_y & \beta_u \lambda_z \\ \gamma_l \lambda_x & \lambda_y & \alpha_u \lambda_z \\ \beta_l \lambda_x & \alpha_l \lambda_y & \lambda_z \end{bmatrix}. \quad (19)$$

Diagonal extensions (not equal to principal stretches, in general) are $\lambda_x, \lambda_y, \lambda_z$; normalized simple shears are $\alpha_u, \beta_u, \gamma_u$ in upper-triangular off-diagonal positions and $\alpha_l, \beta_l, \gamma_l$ in lower-triangular off-diagonal positions. More precisely, α, β , and γ are the extents of shearing taking place in the 23, 13, and 12 coordinate planes, respectively, with subscripts $(\cdot)_u$ and $(\cdot)_l$ designating their upper- and lower-triangular contributions, respectively.

According to Algorithm 2, for reindexing Case 1 (the user's case):

$$[P_{ij}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \therefore [F_{ij}] = \begin{bmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{bmatrix}; \quad (20a)$$

For reindexing Case 2:

$$[P_{ij}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \therefore [F_{ij}] = \begin{bmatrix} F_{11} & F_{13} & F_{12} \\ F_{31} & F_{33} & F_{32} \\ F_{21} & F_{23} & F_{22} \end{bmatrix}; \quad (20b)$$

For reindexing Case 3:

$$[P_{ij}] = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \therefore [F_{ij}] = \begin{bmatrix} F_{22} & F_{23} & F_{21} \\ F_{32} & F_{33} & F_{31} \\ F_{12} & F_{13} & F_{11} \end{bmatrix}; \quad (20c)$$

For reindexing Case 4:

$$[P_{ij}] = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \therefore [F_{ij}] = \begin{bmatrix} F_{22} & F_{21} & F_{23} \\ F_{12} & F_{11} & F_{13} \\ F_{32} & F_{31} & F_{33} \end{bmatrix}; \quad (20d)$$

For reindexing Case 5:

$$[P_{ij}] = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \therefore [F_{ij}] = \begin{bmatrix} F_{33} & F_{31} & F_{32} \\ F_{13} & F_{11} & F_{12} \\ F_{23} & F_{21} & F_{22} \end{bmatrix}; \quad (20e)$$

For reindexing Case 6:

$$[P_{ij}] = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \therefore [F_{ij}] = \begin{bmatrix} F_{33} & F_{32} & F_{31} \\ F_{23} & F_{22} & F_{21} \\ F_{13} & F_{12} & F_{11} \end{bmatrix}. \quad (20f)$$

The determinant of matrix $[P_{ij}]$ is +1 for Cases 1, 3, and 5, and -1 for Cases 2, 4, and 6.

For the three pairs of off-diagonal terms, viz., (F_{12}, F_{21}) , (F_{13}, F_{31}) , and (F_{23}, F_{32}) , there are eight possible combinations for placing the maximum of each pair into an upper-triangular location, normalized for their extents of shear. However, there are only six possible permutation cases by which such coordinate transformations can happen. Consequently, Cases 1 and 6, whose permutation matrices are diagonal in form (cf. Eq. 20), have been selected to place the maximum off-diagonal terms into the nearest sub-diagonal entries of the transformed matrix (i.e., (F_{12}, F_{21}) and (F_{23}, F_{32})), but they cannot assure that the furthest component, viz., that which associates with pair (F_{13}, F_{31}) , has the greatest shear extent, or not. The other four cases assure that all terms in the upper triangle associate with maximum extents of shear. The contributions remaining in the lower-triangular positions therefore associate with three, separate, pure shears, each occurring on a shear plane that is orthogonal to the other two.

As an input to Algorithm 2, matrix $[F_{ij}]$ contains the components of $\mathbf{F}$ evaluated in coordinate system (i, j, k) , as defined in tensor form in Eq. 1 and interpreted in the user's frame in Eq. 19. As an output from Algorithm 2, matrix $[F_{ij}]$ contains the components of $\mathbf{F}$ in a permuted coordinate system with base vectors $(\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3)$ (i.e., the physical coordinate system, prior to Gram rotation, used in our analysis of a dodecahedron¹⁷).

Base vectors map according to Eq. 4, while vector and matrix components map according to Eq. 7c. There is no rotation or stretching of the coordinate axes during this process, only a possible relabeling of them.

The overarching strategy, per Conjecture 1, is to place those extents of shear with the greatest magnitudes into upper-triangular matrix locations via an appropriate coordinate permutation, which is what Algorithm 2 does. Consequently, the shear terms in the resulting lower-triangular matrix locations are handled as pure shears in their respective planes, while the resulting upper-triangular matrix locations contain these pure shears, possibly combined with attributes of simple shear.

The pure shears associate with a Gram rotation of physical base vectors $(\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3)$ into physical base vectors $(\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3)$. The latter, namely $(\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3)$, compose a coordinate frame in which 3-D Laplace stretch components $(a, b, c, \alpha, \beta, \gamma)$ of Eq. 3 can be measured explicitly.⁴ Scalar strain attributes obtained from components of the Laplace stretch, and their work-conjugate scalar stress measures, are then used

in constitutive models developed in detail elsewhere.^{4,5} It is in either of coordinate systems $(\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3)$ or $(\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3)$, where all constitutive equations are to be formulated for the parenchyma,^{12–14,17} against which the lung constitutive theories in our FE models are referenced.^{15,16}

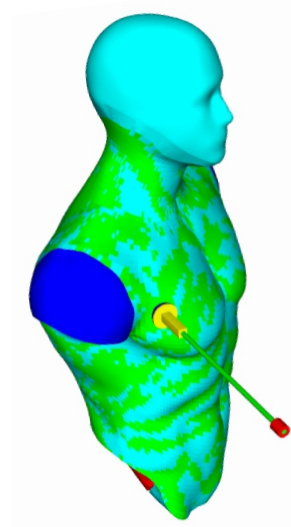
4. Deformation Gradient Histories from Dynamic Simulations

Results of new and existing¹⁶ FE simulations of dynamic impact to the human torso are used to exercise and evaluate efficacy of the new indexing procedures set forth for 3-D analysis in Section 3.2. Deformation gradient histories are required; their acquisitions from existing FE simulation results are discussed in Section 4.

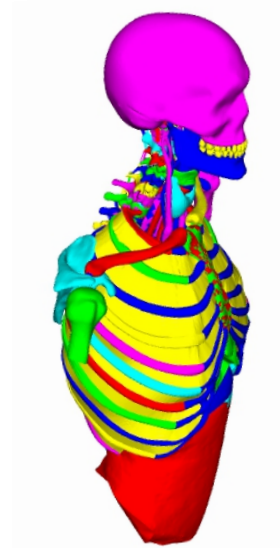
4.1 Torso Impact Protocols

The FE model of the human torso and head implemented in LS-DYNA is known as the Advanced Total Body Model Version 2.5 (ATBM 2.5). The complete model consists of the FE mesh, constitutive behaviors, material properties, and simulation control parameters (e.g., contact and hourglass settings) for the human torso. Skin, muscle, connective tissue, the skeletal system, and internal organs, among other features, are all resolved explicitly. Library constitutive models available in LS-DYNA are used, consisting of linear elastic, nonlinear elastic, plastic, or viscoelastic materials depending on the particular biological constituent. The original ATBM 2.5 uses a low-density foam constitutive law²³ for the lungs. In the work reported by Clayton et al.,¹⁶ from which local deformation gradient histories are extracted in what follows, the foam constitutive law is replaced with the nonlinear material model described in prior work.^{12–15} A complete description of the other features (e.g., specific properties and parameters) of the ATBM 2.5 is outside the present scope. Various components of the geometry are visualized in Fig. 5.

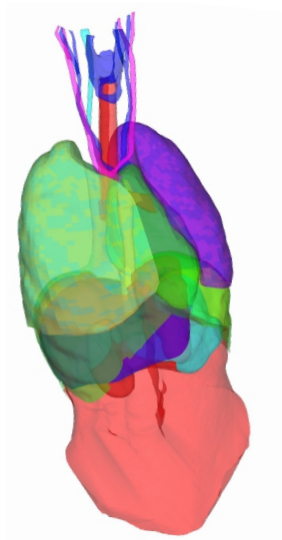
The projectile²⁴ used in torso impact simulations¹⁶ is a stiff impactor instrumented with a wired accelerometer. The striking end is covered by a 40-mm-diameter solid hemisphere made from a plastic material. This hemisphere, which inhibits perforation of the torso for high-impact velocities, is fastened to an aluminum housing that contains the accelerometer. The housing is connected to a long aluminum pushrod whose back end is fixed to a plastic cylinder that fits in the barrel of a pressurized launcher. The total mass of the FE representation of the projectile, created at the US Army Combat Capabilities Development Command Army Research Labora-



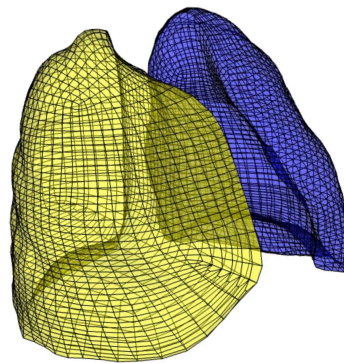
(a) external view & rod



(b) skin & flesh removed



(c) internal organs



(d) lungs

Fig. 5 Human ATBM 2.5¹⁶: a) entire model including projectile, b) skull and torso with skin and flesh removed for visualization, c) torso with skin, flesh, and skeletal system removed for visualization, and d) lungs with hexahedral mesh

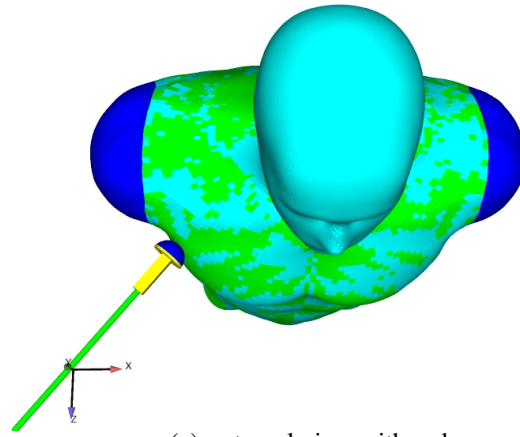
tory, is 72.3 g. Numerous simulations are reported in prior work¹⁶: impact velocity and several other parameters are varied among many described simulations therein. The LS-DYNA code²³ is used, where the constitutive behavior of the lung is modeled according to the theory of Clayton and Freed,^{12,13} computer implementation of Clayton et al.,^{15,16} and parameterization for human lung tissue of Clayton et al.¹⁶

The rod strikes the torso in the right upper chest region, as evident in Fig. 5a. For results utilized herein, the rod impact velocity, denoted as v_I , is prescribed as 90 m/s. Corresponding kinetic energy (KE) of the rod is 292.8 J. Analogous experiments on live pigs²⁴ with $v_I \in [35, 95]$ m/s suggest that a threshold impact velocity of around 75 m/s exists, where lung injuries are usually observed for most velocities above and are usually not observed for most velocities below. This threshold corresponds to a projectile KE of around 200 J. Injuries sustained by two human patients struck by nonlethal projectiles (rubber bullets) with KEs around 200 J were evaluated in a different study.²⁵ In that work, one of the two patients suffered heart and lung contusion requiring hospitalization. These prior studies suggest that the projectile modeled in Clayton et al.¹⁶ with impact velocity of 90 m/s would induce severe lung injury in a human subject.

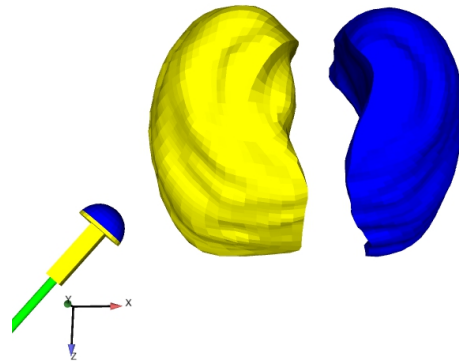
Deformation gradient histories in the observer's frame, $F_{ij}(X_k, t)$, are extracted over a time period $t \in [0, 34]$ ms from LS-DYNA simulations reported by Clayton et al.¹⁶ The fixed increment between extracted data points is $h = 0.1$ ms, which is notably larger than the variable simulation time step, constrained by Courant's condition,^{23,26} used to explicitly integrate the balances of linear momentum and energy. In the simulation, the right lung bears much more deformation than the left lung, so deformation histories are extracted only for the right lung.

The initial orientation of the rod with respect to the torso and lungs is shown in Fig. 6. Coordinates X_k and basis vectors $(\mathbf{i}, \mathbf{j}, \mathbf{k})$ in what follows correspond to the observer's frame (i.e., that of the experimentalist). The horizontal direction pointing from the chest towards the left arm is $+X_1$. The vertical direction, parallel to the spine and positive from torso to the head, is $+X_2$. The horizontal direction pointing from the spine to the front of the chest wall is $+X_3$.

Define unit vectors $(\mathbf{i}, \mathbf{j}, \mathbf{k})$ parallel to respective $(X_1, X_2, X_3) \leftrightarrow (X, Y, Z)$ Cartesian directions. In this laboratory coordinate frame, the initial velocity vector of the projectile is $\mathbf{v}_I = \frac{1}{\sqrt{2}}v_I(\mathbf{i} - \mathbf{k})$. Much, but not all, of the impulse imparted to the



(a) external view with rod



(b) extracted lungs with rod

Fig. 6 Quantities referred to user/laboratory coordinate system (i,j,k) for human ATBM 2.5¹⁶:
 a) initial conditions, top view, entire model including projectile and b) initial conditions, top view, extracted lungs (right:=yellow, left:=blue) and projectile

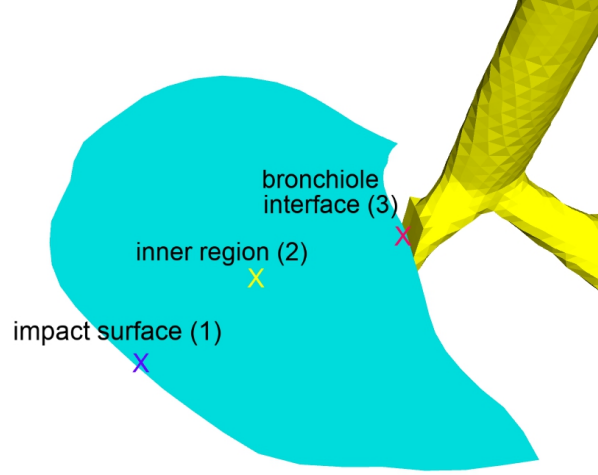


Fig. 7 Human ATBM 2.5¹⁶: cross section of right lung in XZ plane with bronchiole tube (right) and three locations for deformation gradient history extraction

lung leads to compression in the X_1 direction.

4.2 History Data

Deformation gradient histories are obtained for three locations located within the same vertical cross section ($X_2 = Y = \text{constant}$) in the right lung, as shown in Fig. 7. Location 1 is near the pleural surface and is very close to the point of impact that occurs external to the chest wall. Location 2 is centrally located within the right lung. Location 3 is farthest from the impact site and is adjacent to a bronchiole tube resolved by the FE mesh of the ATBM. In the LS-DYNA simulations, 8-node solid hexahedral elements with reduced integration²³ are used to represent the lungs. Extracted values thus correspond to a finite element with a single integration point (i.e., Gauss point) at reference location X .

Deformation gradient histories are plotted in Figs. 8–16. The determinant of the deformation gradient $\det[\mathbf{F}_{ij}] = \det \mathbf{F}$ is plotted in Fig. 17. Deformation initiates earliest at location 1, followed secondly by location 2, and lastly in location 3. Initiation times of significant deformation at each location are consistent with transit times of longitudinal stress waves through the highly deformed FE mesh.

The primary component of compression at each location is F_{11} . Local volume change as measured by $\det \mathbf{F}$, which is invariant under reindexing and all rotation operations, is most severe closest to the impact site (i.e., location 1), but all

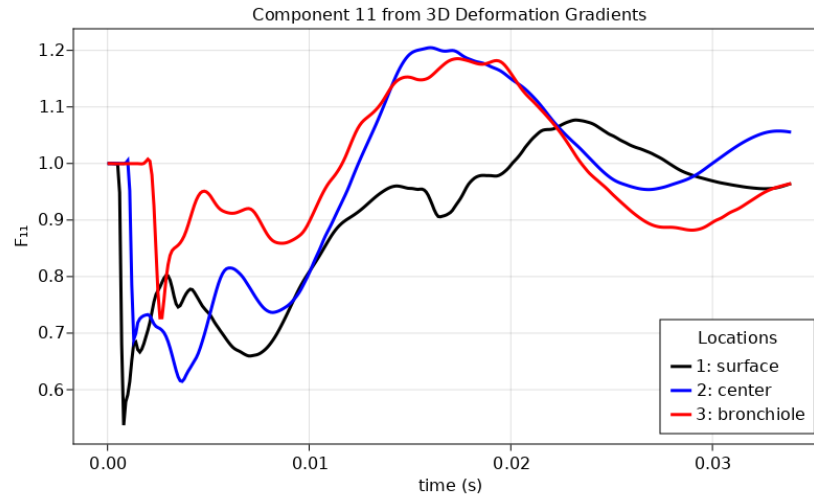


Fig. 8 History of deformation gradient component F_{11} at three locations in right lung extracted from LS-DYNA simulations of human torso impact¹⁶

deformation gradient components can attain large magnitudes at all three locations depending on the time instant resolved. At every location, strain and rotation can be finite, demonstrating necessity of a geometrically nonlinear constitutive description.¹²⁻¹⁴

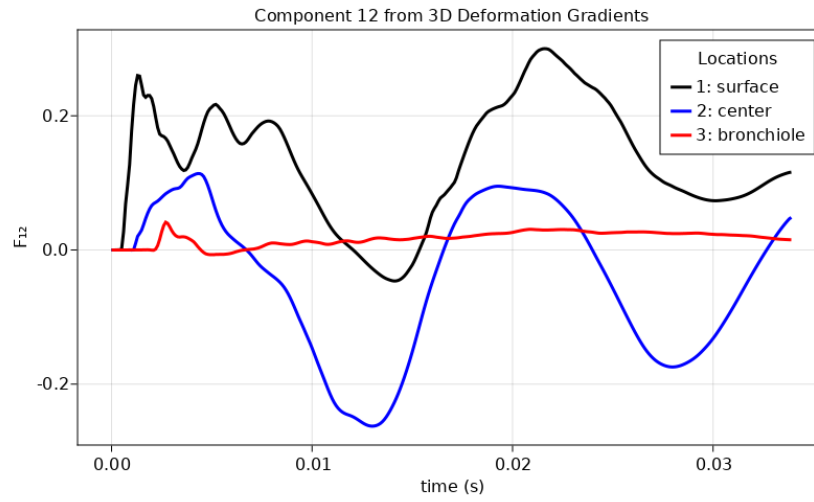


Fig. 9 History of deformation gradient component F_{12} at three locations in right lung extracted from LS-DYNA simulations of human torso impact¹⁶

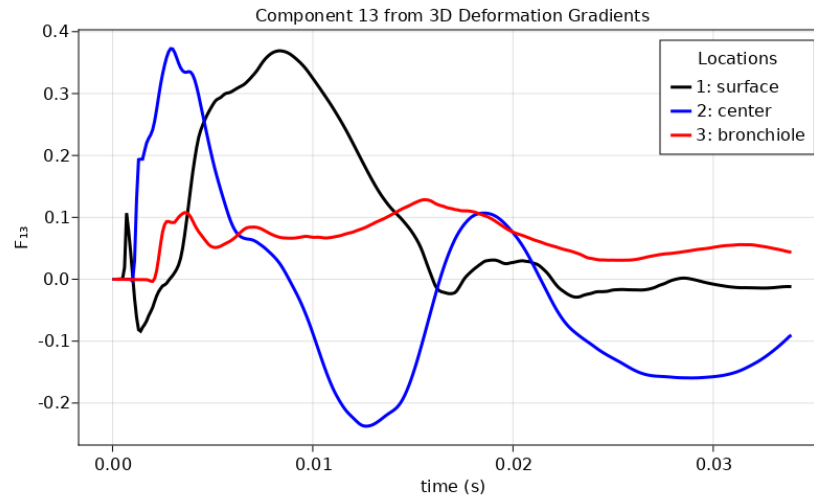


Fig. 10 History of deformation gradient component F_{13} at three locations in right lung extracted from LS-DYNA simulations of human torso impact¹⁶

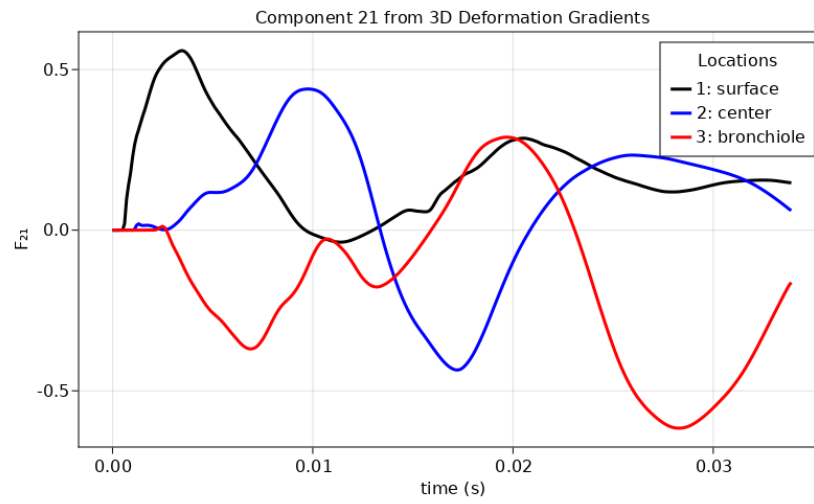


Fig. 11 History of deformation gradient component F_{21} at three locations in right lung extracted from LS-DYNA simulations of human torso impact¹⁶

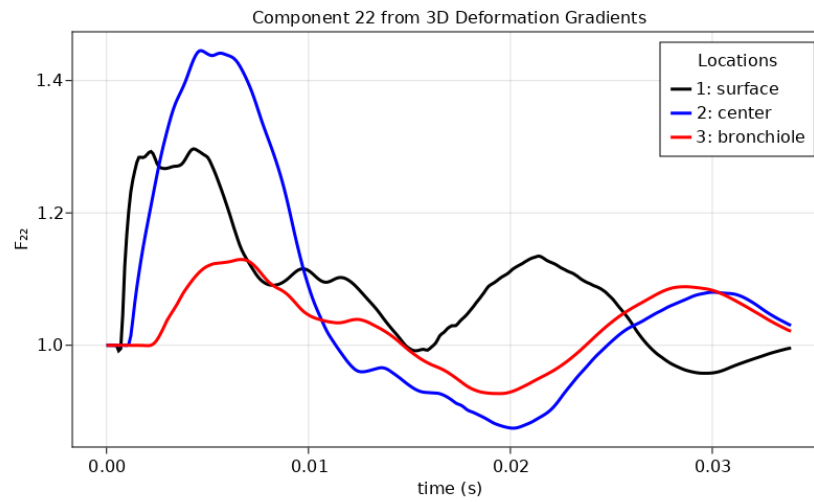


Fig. 12 History of deformation gradient component F_{22} at three locations in right lung extracted from LS-DYNA simulations of human torso impact¹⁶

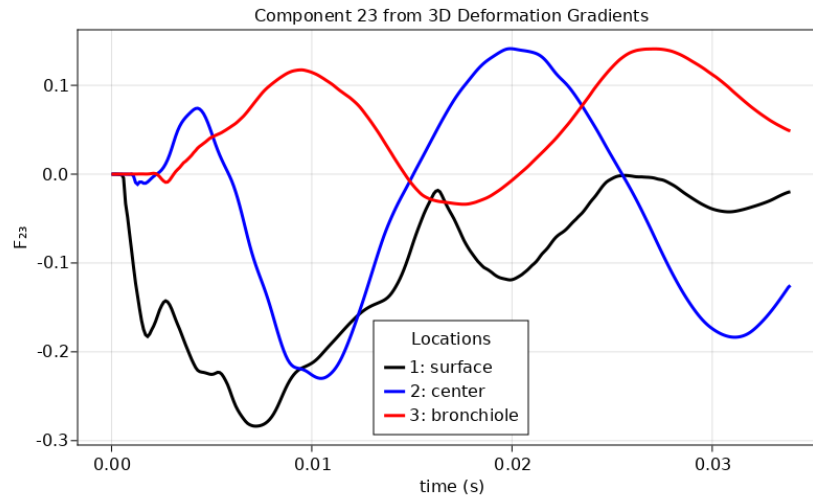


Fig. 13 History of deformation gradient component F_{23} at three locations in right lung extracted from LS-DYNA simulations of human torso impact¹⁶

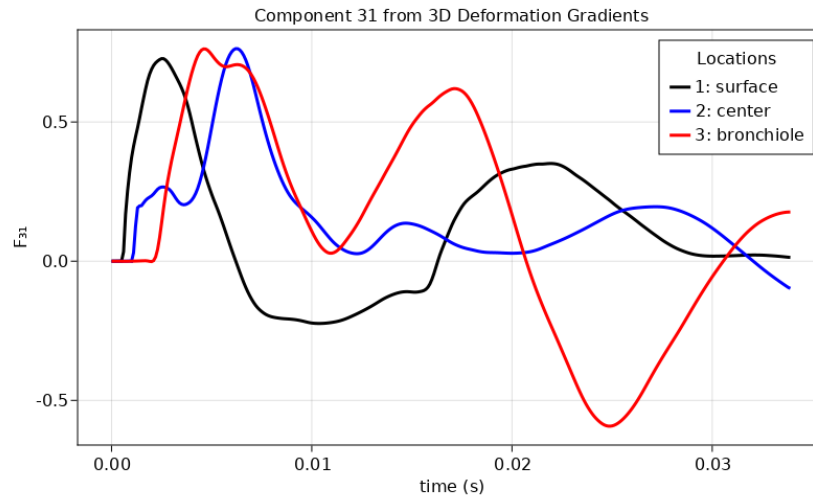


Fig. 14 History of deformation gradient component F_{31} at three locations in right lung extracted from LS-DYNA simulations of human torso impact¹⁶

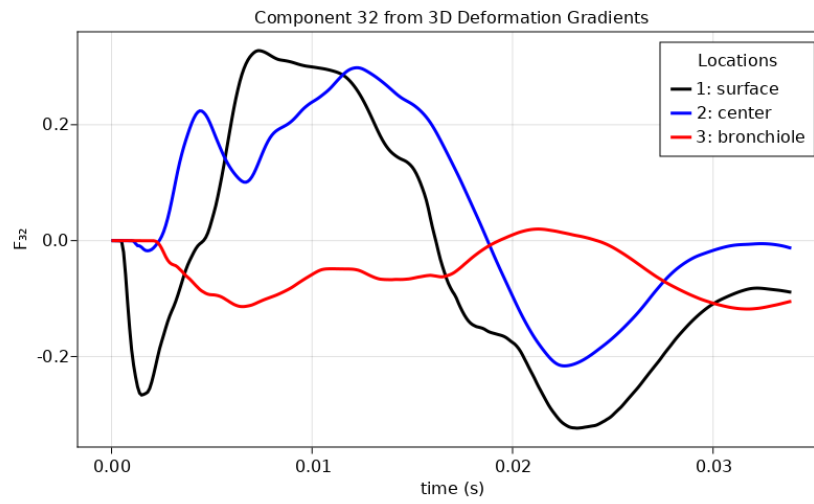


Fig. 15 History of deformation gradient component F_{32} at three locations in right lung extracted from LS-DYNA simulations of human torso impact¹⁶

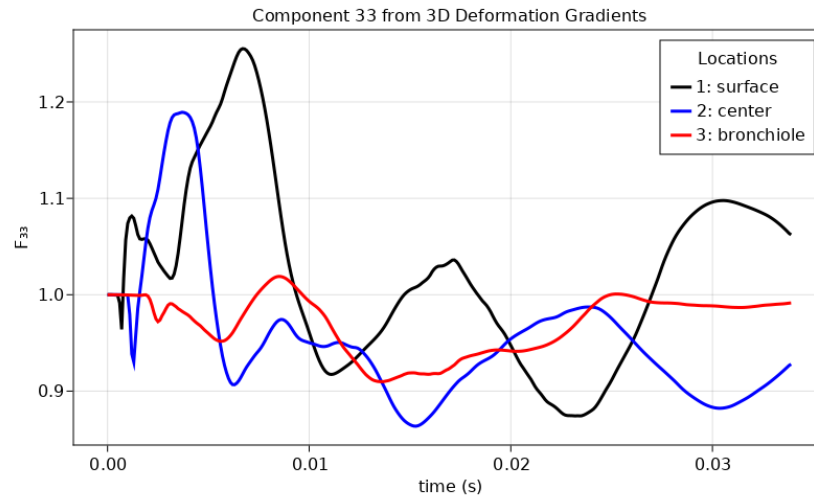


Fig. 16 History of deformation gradient component F_{33} at three locations in right lung extracted from LS-DYNA simulations of human torso impact¹⁶

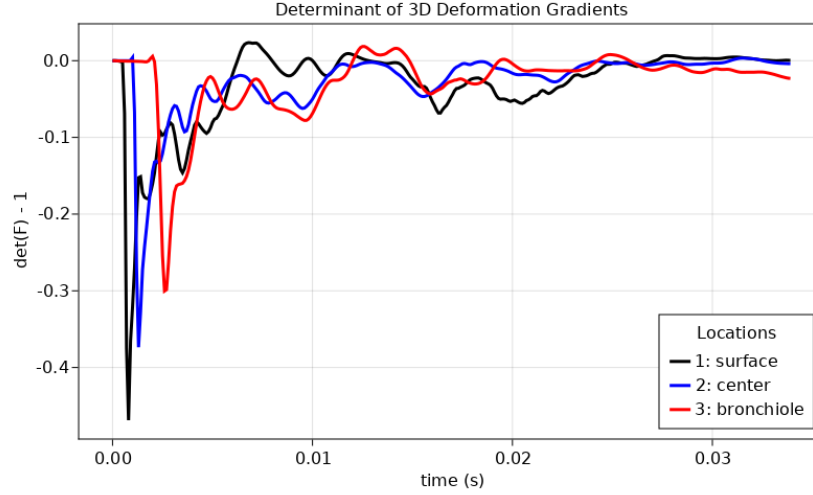


Fig. 17 History of deformation gradient determinant $\det \mathbf{F} = \det[\mathbf{F}_{ij}] = \det[\mathbf{F}_{ij}] = abc$ at three locations in right lung extracted from LS-DYNA simulations of human torso impact¹⁶

5. Evaluation of Indexing Strategies

Previous and new methods for coordinate indexing in the context of 3-D numerical simulations of torso impact are described. Results of prior¹⁶ and new FE simulations invoking the different methods are then analyzed.

5.1 Methods

Advantages and disadvantages of the dynamic indexing method of Freed and Zamani⁴ and Paul et al.¹⁹ are summarized. The stationary (i.e., static) indexing technique of Section 3.2 of the current work is then similarly assessed. For the latter, the appropriate pivoting case per Algorithm 2 is identified according to data presented in Section 4.2.

5.1.1 Dynamic Indexing

The original simulations of Clayton et al.¹⁶ invoke dynamic pivoting, whereby coordinate basis vectors are potentially reindexed⁴ using the algorithm for Lagrangian Laplace stretch presented in detail by Paul et al.¹⁹ Reindexing is applied transiently and pointwise, following physically motivated criteria described by Paul et al.¹⁹ This strategy intends to alleviate possible dependence of predicted stress

attributes—in the context of a constitutive model based on strain attributes derived from the Laplace stretch^{4,5,12,13}—on the selection of basis vectors (i, j, k) made, perhaps arbitrarily, by an external observer.

As shown by Paul et al.,¹⁹ this method of dynamic indexing preserves continuity of Laplace stretch components $(a, b, c, \alpha, \beta, \gamma)$ in Eq. 3 during pivoting operations. Therefore, stress components in hyperelastic models^{5,12,13,15} conjugate to strain attributes culled from Laplace stretch should also remain continuous upon such dynamic reindexing. This strain continuity then provides continuity of the stress tensor when referred to the Gram-rotated physical basis $(\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3)$. On the other hand, Gram rotation $\mathbf{R}$ is not necessarily continuous upon dynamic pivoting according to the algorithm of Paul et al.¹⁹ Discontinuities in $\mathbf{R}$, in turn, would lead to discontinuities in the Cauchy stress tensor referred to the physical basis $(\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3)$ according to Eq. 8. Discontinuities in pivoting matrix components $[P_{ij}]$ would instill further discontinuities in Cauchy stress referred to the user's basis (i, j, k) according to Eqs. 4a or 4b.

If the off-diagonal components of the deformation gradient F_{ij} ($i \neq j$) of a material element change in certain ways during the history of motion, transient reindexing can induce abrupt yet continuous changes in Laplace stretch components, as well as discontinuities in components of Gram rotation. Discontinuities in Cauchy stress components are then possible. Such discontinuities are likely unphysical, though their severity would depend on the particular material model and particular deformation histories in question. The partitioning of strain into squeeze versus simple shearing modes can be altered by coordinate reindexing, which can lead to rapid transients, but not discontinuities, in strain energy density.

Volume is invariant with respect to coordinate indexing, as is Cauchy pressure (i.e., one-third the trace of negative stress), so an isotropic solid with a fully decoupled deviatoric-volumetric response would not demonstrate a discontinuities in its pressure history due to a transient reindexing. In materials that are nearly incompressible (e.g., lung parenchyma under the closed-cell approximation^{12,13}), longitudinal wave propagation should not be severely affected by transient reindexing, but non-negligible shear wave perturbations are conceivable.

Furthermore, one cannot always unfailingly apply Conjecture 1 over an entire deformation history for a general transient boundary value problem (i.e., one featuring

heterogeneous deformation) since the deformation gradient history is not known at each material point a priori.

5.1.2 Stationary Indexing

The simplest possible alternative to the previous, dynamic 3-D strategy of Freed, Paul, and co-workers^{4,16,19} is for the modeler to impose uniform (both spatially and temporally) coordinate indexing, only at the beginning of an analysis. This alternative eliminates above-mentioned rapid transients in Laplace stretch components, since uniform reindexing (or a total lack thereof) does not affect partitioning of deviatoric deformation into simple shear versus squeeze modes abruptly during the history of deformation. Furthermore, temporal discontinuities in R_{ij} and P_{ij} , which would induce discontinuities in deviatoric components of Cauchy stress as discussed in the context of dynamic indexing^{4,19} are avoided by the stationary approach.

However, if the deformation gradient history is unknown, then this strategy is also likely unphysical, because it delegates the choice of P_{ij} and ultimately the coordinate basis vectors $(\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3)$ to the analyst or modeler, rather than imposing a physically motivated algorithm based on kinematic characteristics.¹⁹ By enabling the modeler to explicitly choose a coordinate system that influences predictions of the constitutive model (e.g., one based on Laplace strain attributes^{4,5}), a kind of artificial anisotropy (i.e., directional dependence of response), not necessarily indicative of true material behavior, is essentially introduced into the analysis.

On the other hand, when the deformation gradient history $F_{ij}(X_k, t)$ is known a priori, for example, in problems involving homogeneous deformation under Dirichlet boundary conditions, the methodology of Section 3.2 can be used to provide a unique choice of pivoting matrix $[P_{ij}]$ and thus a unique set of basis vectors $(\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3)$ obtained from the user's basis $(\mathbf{i}, \mathbf{j}, \mathbf{k})$. In these situations, the appropriate case for indexing (cf. Eqs. 20a–20f) is obtained from Algorithm 2. When the relative magnitudes of deformation gradient components fluctuate over time t , then the dominant case is chosen based on the time-averaged components of $[F_{ij}]$ over the history.

As explained in Section 3.2, the general strategy of the new indexing method proposed in the current work is selection of that pivoting matrix $[P_{ij}]$ that maximizes the extent of simple shears in upper-triangular positions, leaving lower-triangular

positions to consist primarily of pure shear contributions. When relative magnitudes of components F_{ij} fluctuate in space X_k as well as time, then averaging of deformation gradient components to apply Algorithm 2 must proceed in space as well as time if an indexing strategy uniform in space-time is to be invoked. In a space-time averaged, but not necessarily local, sense, this stationary indexing procedure produces a basis $(\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3)$ and pivoted deformation gradient matrix $F_{ij}(X_k, t)$ consistent with Conjecture 1.

However, though not pursued further herein, it is possible to apply a spatially non-uniform, but temporally uniform, reindexing. This would avoid abrupt transients in predictions of constitutive models, though emergence of non-physical spatial variations in response predictions across material boundaries over which $[P_{ij}]$ is discontinuous with respect to X_k would seem likely.

As reported in Section 4.2, deformation gradient histories $\{\mathbf{F}(\mathbf{X}, t_0), \mathbf{F}(\mathbf{X}, t_1), \dots, \mathbf{F}(\mathbf{X}, t_N)\}$ have been extracted from a human torso model¹⁶ at discrete times $t_0, t_1, \dots, t_N$ spanning $t \in [0, 34]$ ms, separated by a fixed increment in time of $h = 0.1$ ms so that $N = 340$. Components $F_{ij}(X_k, t_n)$ for these $N + 1$ deformation gradients have been evaluated in the coordinate system (i, j, k) of this FE analysis. These histories of deformation can be used to establish the boundary conditions to be imposed upon our alveolar model in accordance with the local affinity conjecture stated by Freed et al.¹⁷

Cubic B-splines have been used to interpolate the various components of a deformation gradient history using these 340 data points as knots of correlation so that their first and second derivatives in time can be ascertained, which interpolate as quadratic and linear splines, respectively. Splines are drawn with 1000 uniformly spaced nodes spanning the 340 knots of collocation, where representative results for component F_{22} and its first and second time derivatives, $\dot{F}_{22}$ and $\ddot{F}_{22}$ respectively, are shown in Fig. 18.

There are no noticeable differences between the plots of raw data (Fig. 12) and splined data (top graphic in Fig. 18). Arrival of the stress wave is readily apparent in the $\ddot{F}_{ij}$ profiles obtained from analytical derivatives of the cubic splines. Severity of the stress wave diminishes as it propagates over the lung in the FE simulations,¹⁶ which agrees with analytical solutions from continuum mixture theory.¹⁸ Consequently, the greatest damage caused by the simulated impact event ought to occur

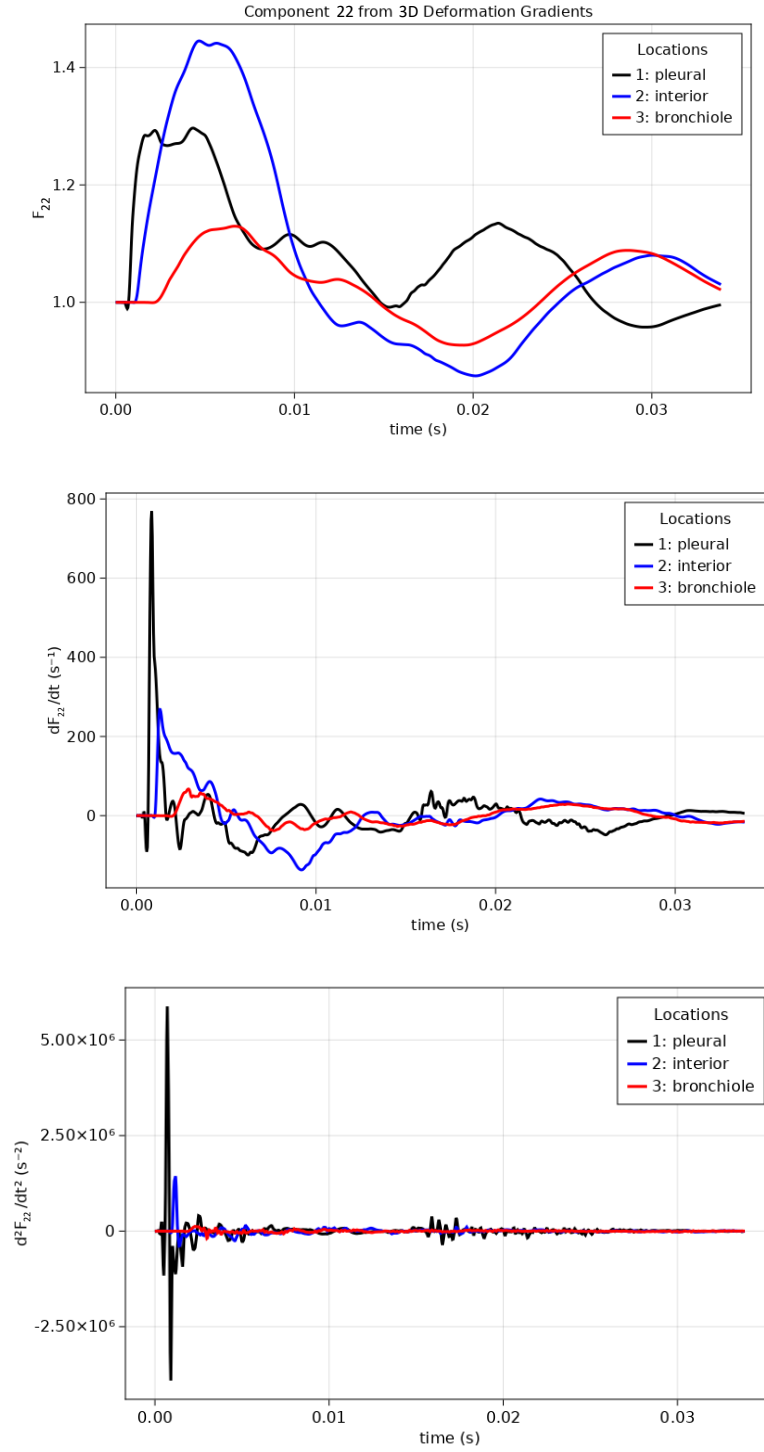


Fig. 18 History of deformation gradient component F_{22} (top) with its first dF_{22}/dt (center) and second d^2F_{22}/dt^2 (bottom) derivatives. A cubic B-spline was used to fit F_{22} so a quadratic spline describes dF_{22}/dt and a linear spline describes d^2F_{22}/dt^2 , all in a coordinate system with base vectors (i, j, k) for the three locations positioned within the right lung of Fig. 7.

near the pleural membrane, which agrees with experimental observations.²⁷

From space-time averaging over all data points (i.e., over all 340 knots) and over all three lung locations in Fig. 7, the averaged extents of shear $\alpha_u, \gamma_u, \beta_u, \alpha_l, \gamma_l, \beta_l$ from Eq. 19 are determined. The space-time averaged magnitudes (i.e., absolute values) are listed in Table 1. The magnitudes for shear in the lower-triangular positions $(\cdot)_l$ are seen to always exceed those of their upper-triangular counterparts $(\cdot)_u$ when evaluated in the (i, j, k) coordinate system. This condition correlates exactly with Case 6 in Algorithm 2. It is noteworthy that the average extents of shear, in all six off-diagonal components of the deformation gradient, are finite in magnitude. Small-strain theory cannot be accurately applied here.

Results in Table 1 imply that lung tissue will shear as much to get out of the way of an impending projectile as it will shear along the direction of a moving projectile; hence, Case 6 applies. Case 6 is also anticipated to apply whenever an analysis considers a Soldier being shot from behind at the same 45° angle relative to directors i and k . Only the signs but not relative magnitudes of the shears would be affected by such a reversal of direction of the projectile in Fig. 6, neglecting any internal geometric changes and anisotropies of the torso constituents. Following the perceived, but not proven, implication that more shearing will occur in directions normal to the axis of a directional impact, rather than parallel to it, Case 1 is anticipated to apply whenever an analysis pertains to a Soldier being struck directly from the side.

Shown in Fig. 19 are the transient histories, at all three locations of Fig. 7, of that Case that would be obtained from Algorithm 2 were the associated pivoting scheme to be applied dynamically and distinctly at each spatial location. Temporal discontinuities in case selection, and hence temporal discontinuities in $[P_{ij}]$, are obvious at all three locations. Furthermore, at fixed t , the local case can vary among each spatial position, suggesting spatial discontinuities in $[P_{ij}]$ as well. All such discontinuities are avoided when the time- and position-averaged shears are used to assign a stationary pivoting matrix, though Conjecture 1 is satisfied only in a globally averaged sense and is locally violated when cases other than Case 6 are suggested.

Predictions of the lung constitutive model used in Clayton et al.,¹⁶ at impact velocity $v_I = 90$ m/s, are now reexamined using three different pivoting strategies:

- Dynamic indexing with the algorithm of Paul et al.,¹⁹ with $[P_{ij}(X_k, t)]$ non-

Table 1 Position-time-averaged absolute values of shear (normalized off-diagonal F_{ij} components of Eq. 19) recorded over all three locations of Fig. 7 within impacted lung from FE simulations¹⁶

Component	Magnitude
α_u	9.19×10^{-2}
β_u	9.91×10^{-2}
γ_u	7.85×10^{-2}
α_l	1.18×10^{-1}
β_l	2.58×10^{-1}
γ_l	2.24×10^{-1}

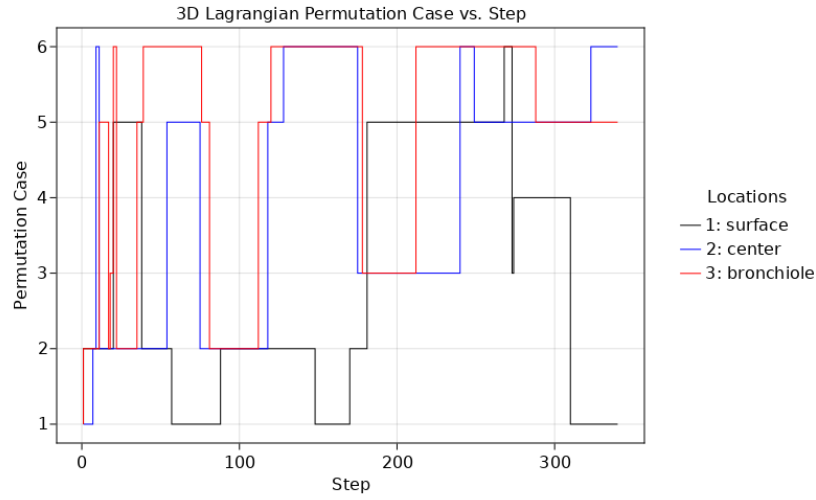


Fig. 19 Cases for permutation from coordinates (i, j, k) into coordinates (E_1, E_2, E_3) to ensure frame-indifferent Laplace kinematics for Lagrangian analyses given the deformation gradient components F_{ij} presented in Figs. 8–16. All six cases have regions of applicability over this deformation history.

uniform in both space and time as in the original work¹⁶ and recapitulated in Section 5.1.1.

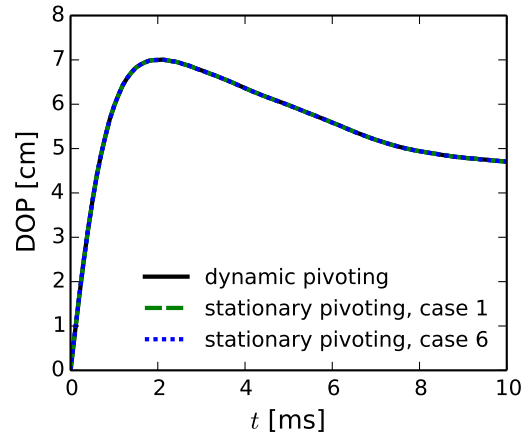
- Stationary indexing by applying Case 6 of Eq. 20f as motivated by the data analysis of Section 5.1.2 and application of Algorithm 2 to averaged shears in Table 1, whereby the constant pivoting matrix $[P_{ij}]$ is imposed a priori as $[0\ 0\ 1; 0\ 1\ 0; 1\ 0\ 0]$.
- Uniform, null pivoting by applying Case 1 of Eq. 20a, whereby the pivoting matrix $[P_{ij}]$ degenerates to the identity $\text{diag}(1, 1, 1)$, essentially leaving the laboratory system unchanged.

New FE simulations are undertaken to obtain new results when the second and third strategies are invoked, since these stationary indexing schemes were not implemented in prior works. Outcomes of different torso impact simulations invoking all three strategies (though only one method per individual FE simulation) are analyzed in what follows.

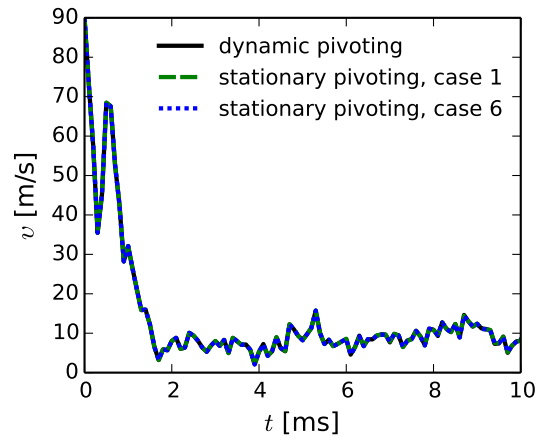
5.2 Results

Shown in Fig. 20a for all three pivoting strategies is the depth of penetration (DOP) of the projectile nose, estimated by the magnitude of displacement of the node at the projectile's tip for $t \leq 10$ ms. Note that the torso is not perforated, so this DOP measures surface displacement rather than piercing of the target as in standard ballistic experiments on armor materials, for example. The corresponding history of velocity magnitude for the projectile's tip is shown in Fig. 20b. Prescription of dynamic versus stationary indexing has no apparent effect on the history of DOP or projectile tip velocity, nor does prescription of uniform indexing with Case 1 versus Case 6.

Similar trends apply for the relative volume occupied by the right lung for each indexing strategy, as shown in Fig. 21. Here, the current (deformed) volume of the right lung is denoted by $V(t)$, while the initial volume is $V_0 = V(0) = \text{constant}$. Volume decreases as a result of the compression process during projectile impact, then expands upon release, with nearly complete elastic recovery ($V \rightarrow V_0$) at late solution times. It is concluded that the gross mechanical response of the lung, in these simulations, is relatively unaffected by the choice of indexing scheme.



(a) projectile tip displacement



(b) projectile tip velocity

Fig. 20 History of a) DOP and b) projectile tip velocity (v) from LS-DYNA simulations of torso impact using three pivoting strategies (results nearly indistinguishable among three strategies)

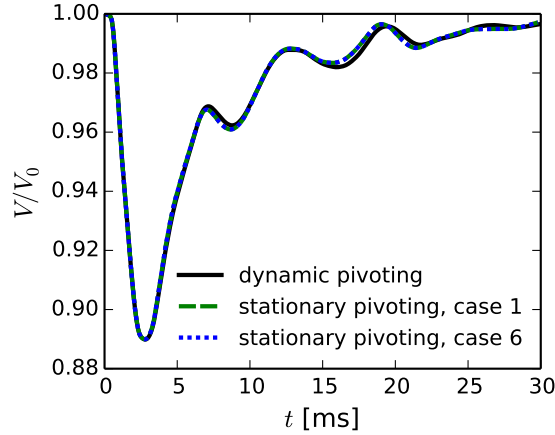
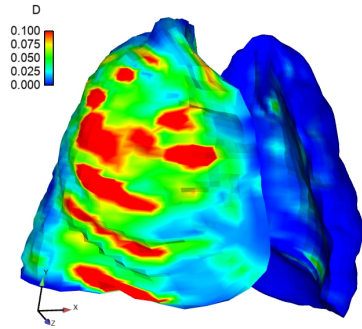


Fig. 21 History of normalized right lung volume V/V_0 from LS-DYNA simulations of torso impact using three pivoting strategies

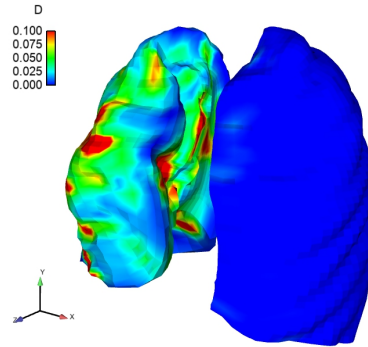
The contours of the damage-injury variable D predicted by the constitutive model of Clayton et al.^{12,13,15,16} are shown in Fig. 22 for each choice of coordinate indexing, at $t = 20$ ms after initial impact. The constitutive model for damage kinetics implemented in dynamic FE simulations^{15,16} contains an amplification factor ω_D enabling more severe injury at higher strain rates. The larger the value of ω_D , the faster the local rate of increase of D with the local rate of increase of internal energy. Notice that the scale of the figure is capped at $D = 0.1$ pertinent to parameter assignment $\omega_D = 0.5$,^{15,16} though the full admissible range is $D \in [0, 1]$. The deformed shape of the lung is very similar regardless of pivoting method. Prescription of stationary indexing with Case 1 and with Case 6 produces very similar D -contours.

Conversely, dynamic pivoting leads to predictions of significantly more severe damage relative to stationary pivoting. The volume average of D over the domain of *both* lungs, denoted as D_V is reported versus simulation time in Fig. 23, confirming this assertion. Stationary indexing methods via Case1 and Case 6 produce extremely similar results for $D_V(t)$. Dynamic reindexing produces 2 to 3 times larger instantaneous values of D_V than static indexing for $t \geq 10$ ms.

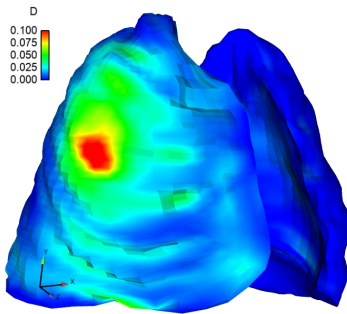
The dynamic method produces greater rates of change of local strain energy density when bases $(\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3)$ are dynamically reindexed, leading to an increased rate-dependent driving force¹⁵ for D . Ridges of relatively large D are evident on the surface of the right lung in Fig. 22a, perhaps where interactions with the much stiffer ribcage occur.



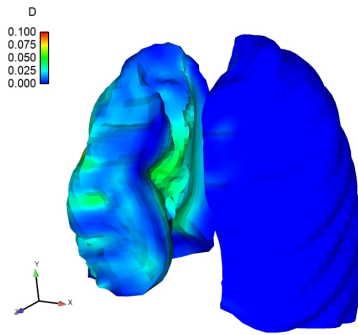
(a) dynamic



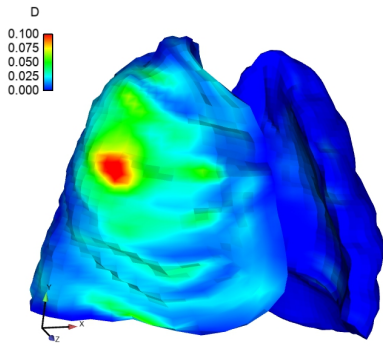
(b) dynamic



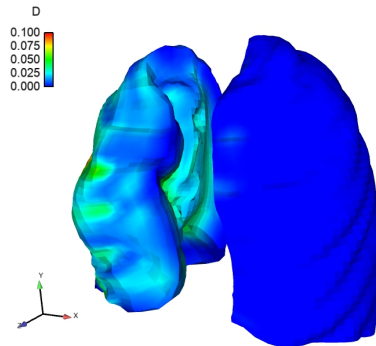
(c) Case 1



(d) Case 1



(e) Case 6



(f) Case 6

Fig. 22 Damage-injury variable in lungs for human ATBM 2.5¹⁶: a) dynamic pivoting, right lung view, b) dynamic pivoting, left lung view, c) uniform pivoting, Case 1, right lung view, d) uniform pivoting, Case 1, left lung view, e) uniform pivoting, Case 6, right lung view, and f) uniform pivoting, Case 6, left lung view

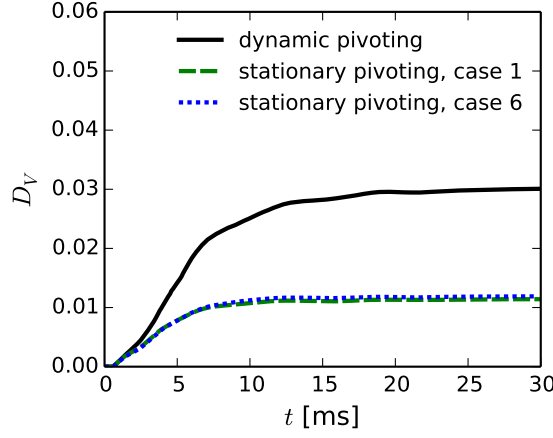


Fig. 23 History of average damage-injury metric $D_V(t) = \frac{1}{V_0} \int D(X, t) dV_0$ from LS-DYNA simulations of torso impact using three pivoting strategies

The current results suggest, that to obtain similar predictions of D , a smaller value of ω_D should be used when the dynamic indexing method^{4,19} is prescribed, and a relatively larger value of ω_D should be used when the stationary indexing method advocated in Section 3.2 of the current work is implemented. As explained in prior work,^{15,16} precise calibration of ω_D requires substantially more experimental data relating local injury to controlled conditions under dynamic impact than are presently available.^{28–30} Methods for quantifying local injury in contemporary lung impact experiments³¹ that seek to provide such data are presently under development.

6. Conclusions

New features of a novel theory for finite-deformation continuum mechanics incorporating an upper-triangular (i.e., QR) factorization of the deformation gradient have been developed and implemented. Reference, initial, and current configurations of a material body have been formally distinguished. The analyst’s frame of reference can, but does not always, differ from the observer’s frame as a result of coordinate indexing. A Lagrangian Gram–Schmidt decomposition has been incorporated. This separates the deformation gradient in the analyst’s frame into a rotation and upper-triangular matrix known as Laplace stretch.

For a given orthonormal triad, the labeling of axes that associates Gram rotation with only pure shears has been conjectured as the appropriately indexed (i.e., po-

tentially pivoted) coordinate basis from which to obtain the Laplace stretch tensor by QR factorization. For temporally and spatially inhomogeneous 3-D problems, a single “stationary” labeling has been proposed to enable closest agreement with this properly indexed basis over the history of states. New algorithms for coordinate indexing in two and three spatial dimensions have been developed to satisfy this conjecture. Components of the space-time averaged deformation gradient measured in the observer’s frame are used for selection of one of among six possible cases for coordinate reindexing. If the deformation gradient history is unknown a priori, however, then invariance is broken in a certain sense since the modeler must manually choose the pivoting matrix, and thus the indexed basis, for subsequent QR factorization.

The new stationary indexing method has been implemented in a lung constitutive model for simulations of dynamic impact to the human torso. Comparisons with prior results invoking dynamic indexing over the history of states show that predictions of local injury are less severe when the new method is used with remaining constitutive parameters unchanged from those used in former studies. The gross mechanical response, for example, projectile penetration depth, projectile tip velocity, and volume change of the impacted lung, is negligibly influenced by the choice of indexing scheme for the present problem.

The earlier-developed dynamic pivoting scheme requires no a priori knowledge of the deformation gradient, and it preserves continuity of Laplace stretch components upon transient reindexing. However, both the Gram rotation matrix and the pivoting matrix demonstrate discontinuities upon reindexing, which can induce discontinuities in deviatoric components of Cauchy stress. Furthermore, abrupt repartitioning of simple and pure shears among continuously varying Laplace attributes can induce rapid transients in local strain energy density that accelerate damage kinetics relative to the new, more stable method. Thus, a smaller value of the parameter modulating rate-dependent damage kinetics should be used for dynamic reindexing than for stationary indexing.

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Appendix A. Input File Syntax for LS-DYNA

The constitutive model of Clayton et al.¹⁶ is implemented as a user subroutine in the LS-DYNA software, version R12.0 (2020). Recommended units (i.e., mass-length-time-force-stress-temperature, not all independent) are **kg-m-sec-N-Pa-K**. The model has only been verified for *ELEMENT_SOLID elements (e.g., shell elements are not supported).

A new, integer-valued parameter $IPIV$ has been added to the original software documented in a previous report.¹⁶ Setting $IPIV = 0$ activates the dynamic pivoting algorithm of Paul et al.¹⁹ discussed in Section 5.1.1 of the current report. Setting $IPIV = 0$ also reproduces conditions that were hard-coded in the original software implementation.¹⁶ Setting $IPIV \in [1, 6]$ activates the stationary (i.e., uniform in space-time) pivoting scheme discussed in Section 5.1.2 of the current report. When $IPIV \in [1, 6]$, the pivoting matrix $[P_{ij}]$ for possible reindexing corresponds to the case number in Eqs. 20a–20f. For example, setting $IPIV = 6$ produces $[P_{ij}]$ for Case 6 in Eq. 20f. As a result of this additional parameter, LMC is now 17 rather than 16 as in the original code.

One possible change to the original set of recommended parameters for human lung¹⁶ is included in the present update. The prescription of $c_2 = 10$ of the original set¹⁶ is now replaced with the flexible range $c_2 \in [10, 60]$. As shown in Appendix B, increasing c_2 provides closer agreement with triaxial extension data, albeit for dog rather than human lung. However, simulations of ballistic impact tend to be more numerically stable when a lower value of c_2 is prescribed, and the value of c_2 has not been validated versus controlled triaxial compression data, which are presently nonexistent. Thus, the user must balance accuracy of tensile predictions (higher c_2 preferred) with stability (lower c_2 preferred) when setting the value of c_2 .

Input is provided through LS-DYNA keyword syntax with the following cards. Alteration of values denoted as “fixed” will likely result in code execution failure. Nonphysical prescriptions of conventionally positive quantities (e.g., zero-valued or negative stiffness moduli) similarly will cause code execution failure.

MAT_050

*MAT_USER_DEFINED_MATERIAL_MODELS

CARD 1

- MID: material identification—unique 8-digit number.

- RO: initial mass density ρ_0 ; must match entry 8 of Card 3.
- MT: material number for user-defined subroutine call (fixed).
- LMC: length of material constant array (total no. entries of Cards 3, 4, and 5).
- NHV: number of user history variables in `hsv` vector (fixed).
- IORTHO: material is not orthotropic (fixed).
- IBULK: Card 3 entry no. of bulk modulus for time step calculation (fixed).
- IG: Card 3 entry no. of shear modulus for time step calculation (fixed).

CARD 2

- IVECT: non-vectorized material model (fixed).
- IFAIL: failure flag not implemented (fixed).
- ITHERM: temperatures implemented (fixed).
- IHYPER: deformation gradient in positions NHV+1 to NHV+9 of `hsv` (fixed).
- IEOS: separate equation of state not used (fixed).

CARD 3

- BD: dynamic closed-cell isentropic bulk modulus $\bar{B}_d^\eta = \bar{B}_0^\eta + \beta_1 B_0^T$.
- GD: dynamic shear modulus $G_d = G_0 \cdot (1 + \beta_3)$.
- C1: exponential bulk stiffening c_1 .
- C2: exponential squeeze stiffening c_2 .
- C3: exponential shear stiffening c_3 .
- GP: ambient pressure derivative of shear modulus $G'_0 = \mu'_0$.
- K0: initial surface tension K_0 .
- RO: initial mass density ρ_0 ; must match entry 2 of Card 1.

CARD 4

- BT: static isothermal bulk modulus $B_0^T \approx B_0^\eta$.
- BETA1: viscoelastic stiffening $\beta_1 = \mu_1/B_0^T = 6G_0\beta_2/B_0^T = G_0\beta_3/B_0^T$.
- CV: specific heat per unit volume at constant volume c_0 .
- GRUN: Grüneisen parameter g_0 .
- Z0: local damage-injury initiation threshold Z_0 (must be nonzero); if $Z_0 < 0$, fully intact stiffness option of Clayton et al.¹⁶ invoked with $Z_0 \rightarrow |Z_0|$.
- ALPHD: damage-injury kinetic coefficient α_D .
- OMEGD: damage-injury kinetic rate amplification ω_D .
- L: mean alveolar diameter l .

CARD 5

- IP IV: pivoting scheme for coordinate indexing; 0 for dynamic or 1, 2, $\dots$, 6 for static Cases 1, 2, $\dots$, 6.

Card 1	1	2	3	4	5	6	7	8
Variable	MID	RO	MT	LMC	NHV	IORTHO	IBULK	IG
Required	user-prescribed	matches Card 3	50	17	6	0	1	2
Type	A8	F	I	I	I	I	I	I

Card 2	1	2	3	4	5	6	7	8
Variable	IVECT	IFAIL	ITHERM	IHYPER	IEOS			
Required	0	0	1	1	0			
Type	I	I	I	I	I			

Card 3	1	2	3	4	5	6	7	8
Variable [units]	BD [Pa]	GD [Pa]	C1 [none]	C2 [none]	C3 [none]	GP [none]	K0 [Pa]	RO [kg/m ³]
Suggested	2.18E+05	7.5E+03	3.0	10.0-60.0	1.0	-0.70	600.0	337.0
Type	F	F	F	F	F	F	F	F

Card 4	9	10	11	12	13	14	15	16
Variable [units]	BT [Pa]	BETA1 [none]	CV [Pa/K]	GRUN [none]	Z0 [none]	ALPHD [none]	OMEGD [none]	L [m]
Suggested	7.5E+03	0.60	7.41E+05	4.91E-04	± 0.64	0.0167	0.5-30.0	1.8E-04
Type	F	F	F	F	F	F	F	F

Card 5	17							
Variable	IPIV							
Required	0 or 1-6							
Type	I							

Appendix B. Lung Constitutive Model Updates

In previous work on constitutive modeling of the lung,¹²⁻¹⁵ potential contributions of squeeze and shear deformations to pressure were linearized without sufficient explanation. A fully nonlinear expression for tensile pressure per unit reference area $\hat{\tau}_0 = -pJ$ that replaces Eq. (3.29)₁ of Clayton and Freed¹² for static loading is

$$\begin{aligned} \hat{\tau}_0 = & (1 - D)B_0^T [\epsilon_0 \exp(c_1 \xi_1^2) - A_0(T - T_0) + \beta_1(\epsilon_0 - \chi_0^1) + K_0/B_0^T \\ & - 3 \frac{\mu'_0}{c_2} \{\exp(c_2 \xi_2) - 1\} - \frac{1}{2} \frac{G'_0}{c_3} \{\exp(c_3 \xi_3) - 1\}]. \end{aligned} \quad (\text{B-1})$$

A fully nonlinear version of Eq. (5.23)₁ of that reference¹² for dynamic loading is

$$\begin{aligned} \hat{\tau}_0 = & (1 - \bar{D}) \{ \bar{B}_0^\eta [\epsilon_0 \exp(c_1 \xi_1^2)] - g_0 T_0 \eta + B_0^T \beta_1(\epsilon_0 - \chi_0^1) + K_0 \} \\ & - (1 - D) B_0^T \left[3 \frac{\mu'_0}{c_2} \{\exp(c_2 \xi_2) - 1\} - \frac{1}{2} \frac{G'_0}{c_3} \{\exp(c_3 \xi_3) - 1\} \right]. \end{aligned} \quad (\text{B-2})$$

Notation is consistent with parameters in Appendix A and is further explained by Clayton and Freed.¹² A similar fully nonlinear version of Eq. (4.34) of Clayton and Freed,⁵ applicable to a more general class of nonlinear hyperelastic solids with exponential stiffening, can be analogously introduced.

The rightmost two terms in each of Eqs. B-1 and B-2 manifest from dependencies of tangent shear moduli on pressure, and hence volume. This in turn yields constitutive coupling of pressure with terms of orders two and higher in shear strain attributes, noting that ξ_2 and ξ_3 are quadratic functions of pure shear strain (i.e., squeeze) and simple shear, respectively.

Corresponding exponential functions for pressure–shear coupling are expanded as the series

$$\frac{1}{c_2} [\exp(c_2 \xi_2) - 1] = \frac{1}{c_2} \left[c_2 \xi_2 + \frac{(c_2 \xi_2)^2}{2!} + \frac{(c_2 \xi_2)^3}{3!} + \dots \right] \approx \xi_2, \quad (\text{B-3})$$

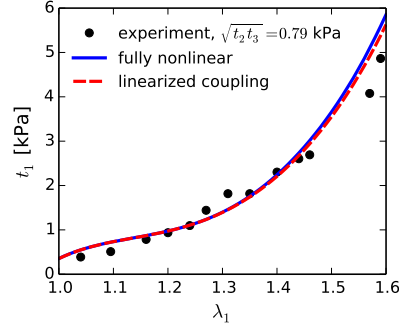
$$\frac{1}{c_3} [\exp(c_3 \xi_3) - 1] = \frac{1}{c_3} \left[c_3 \xi_3 + \frac{(c_3 \xi_3)^2}{2!} + \frac{(c_3 \xi_3)^3}{3!} + \dots \right] \approx \xi_3. \quad (\text{B-4})$$

The rightmost (i.e., linear) approximations were used in prior theoretical work^{12,13,15} and are presently implemented in the LS-DYNA user subroutine documented in Appendix A and a prior report.¹⁶ Clearly, (nonlinear) terms of orders two and higher in ξ_2, ξ_3 are omitted in these rightmost approximations, corresponding to omission of shear strain components of orders four and higher in the pressure.

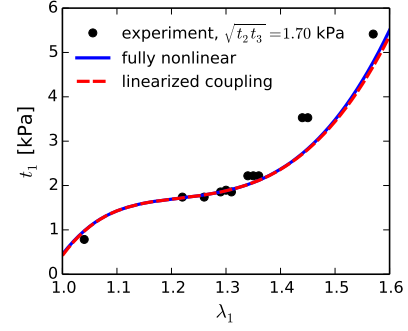
An additional item of note is the choice of dimensionless, nonlinear, pure shear elastic constant c_2 . Original calibration of the constitutive model to triaxial extension data on saline-infused dog lung^{32,33} produced a value of $c_2 = 60$, wherein the approximation of Eq. B-3 was used.¹² Subsequent modeling of human lung tissue under shock compression and ballistic impact¹⁶ suggested a smaller value of $c_2 = 10$. Reducing the value to $c_2 = 10$ was found to greatly improve numerical stability in 3-D finite element simulations,¹⁶ without noticeably affecting the gross mechanical response (e.g., penetration depth versus time) or predictions of local injury (i.e., contours of damage metric D).

New calculations are reported here to assess the ramifications of approximations in Eqs. B-3 and B-4 as well as explore effects of the choice of c_2 . Equations B-1 and B-2 are referred to as the “fully nonlinear” model, while the rightmost approximations in Eqs. B-3 and B-4 are referred to as the “linear coupling” model. The linear coupling model is linear in ξ_1, ξ_2 , meaning it is quadratic (i.e., second-order accurate) in underlying shear strain components. Thus, the linear coupling model is still more sophisticated than classical linear elasticity, which would neglect all coupling between pressure and shear. Note also that the linear coupling model includes the identical contributions of pressure to shear stresses as the fully nonlinear model^{5,12}; differences manifest only in the pressure, and not other (deviatoric) stress components.

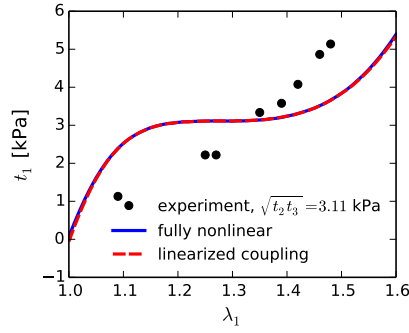
Shown in Fig. B-1 are predictions of principal traction per unit reference area from both models with $c_2 = 60$, for quasi-static triaxial extension loading. Calculation procedures and experimental data are explained further by Clayton and Freed.¹² Shown in Fig. B-2 are predictions of squeeze mode 3 of stress and strain under the same triaxial conditions.¹² Model predictions for $c_2 = 10$ are included for further comparison. Prescription of fully nonlinear versus linear coupling negligibly affects all results. Reducing c_2 from 60 to 10 does, however, affect the $\hat{\tau}_3$ versus ϵ_3 predictions for $|\epsilon_3| \gtrsim 0.1$: at larger shear strains, the increase in tangent stiffness observed experimentally is subdued for $c_2 = 10$.



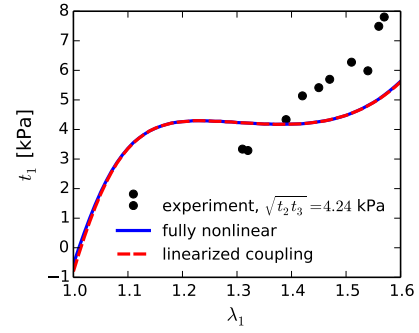
(a)



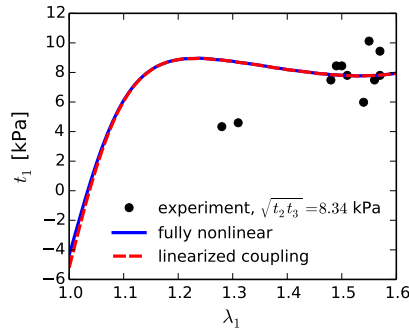
(b)



(c)

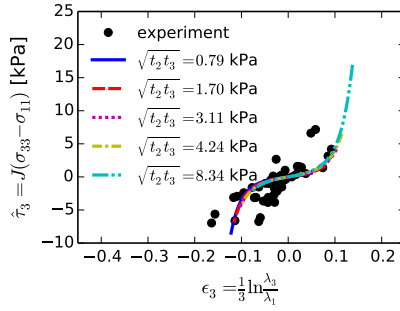


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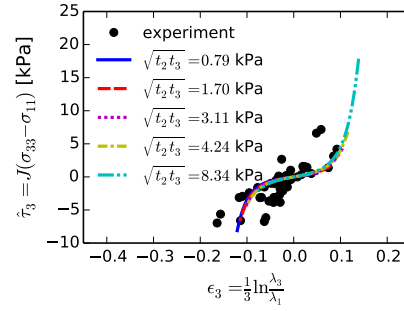


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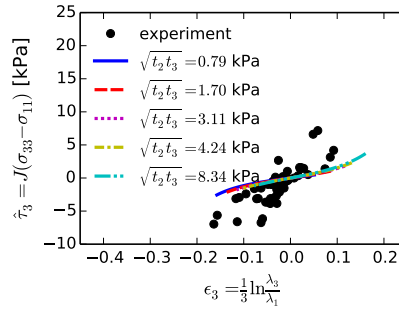
Fig. B-1 Longitudinal traction vs. stretch at different transverse tractions with $c_2 = 60$: fully nonlinear model vs. linearized shear-induced pressure coupling of Clayton and Freed.^{12,13} Calculated results for saline-treated dog lung under triaxial extension are compared to experimental data.³³



(a) fully nonlinear, $c_2 = 60$



(b) linear coupling, $c_2 = 60$



(c) linear coupling, $c_2 = 10$

Fig. B-2 Squeeze mode stress-strain results at different transverse tractions: a) fully nonlinear model with $c_2 = 60$, b) linearized shear-induced pressure coupling^{12,13} with $c_2 = 60$, and c) linearized shear-induced pressure coupling with $c_2 = 10$ as used elsewhere for human lung.¹⁶ Calculated results for saline-treated dog lung under triaxial extension are compared to experimental data.^{32,33}

New calculations for one-dimensional (1-D) shock compression repeat the protocols of Section 6.2 of Clayton and Freed.¹² Results for the linear coupling model used in prior work^{12,13} with $c_2 = 60$ are now augmented with new results of linear coupling with $c_2 = 10$ and of fully nonlinear coupling with $c_2 = 60$.

Hugoniot state predictions are given in Fig. B-3; notation is consistent with Clayton and Freed.¹² Use of fully nonlinear versus linear coupling has no apparent effect. Even with damage kinetics fully suppressed, the difference in P between fully nonlinear and linear coupling is less than 1% for $c_2 = 60$ and $\rho_0/\rho \geq 0.6$. Prescription of c_2 affects shear stress τ for compression $1 - \rho_0/\rho$ greater than 10% and damage D for compression greater than 25%, but c_2 has a relatively minor effect on longitudinal stress P and shock velocity v_s .

The linearization with respect to simple shear in Eq. B-4 does not affect results for triaxial extension or uniaxial compression, since $\xi_3 = 0$ in the absence of simple shear. Linearization in Eq. B-4 does affect pressure predicted under simple shear: see Eq. (4.20)₁ and analysis in Section 4.3 of Clayton and Freed.¹² However, the pressure induced under simple shear was neither reported nor used (e.g., for calibration of c_3) in prior work, so the prior choice of nonlinear versus linear coupling in Eq. B-4 is inconsequential in this regard.

Summarizing current findings, the present analysis suggests that the linear coupling model of Eqs. B-3 and B-4 as used in prior work^{12,13,15} is sufficiently accurate for triaxial extension up to approximately 60% and shock compression up to approximately 30%. The value of c_2 can be reduced from 60 to 10 without significant consequence on longitudinal stress or damage for uniaxial shock compression up to approximately 25%, but shear stress is affected for 1-D compressive strains exceeding 10%.

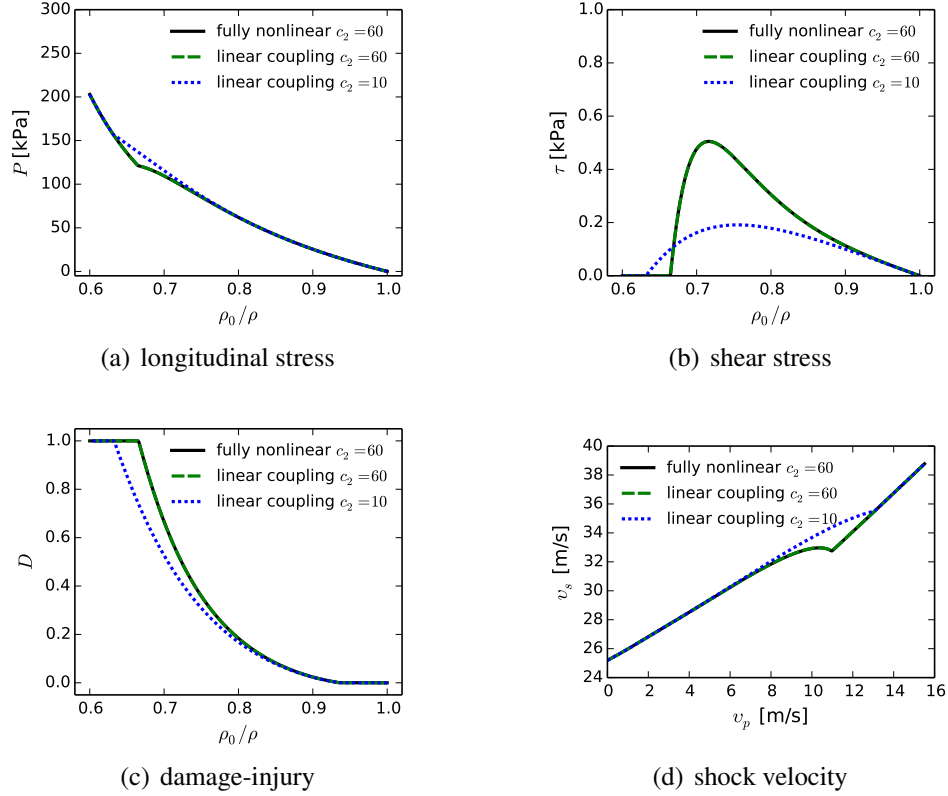


Fig. B-3 Shock Hugoniot response for fully nonlinear model with $c_2 = 60$ vs linearized shear-induced pressure coupling with $c_2 = 60$ as in Clayton and Freed¹² or $c_2 = 10$ as in Clayton et al.¹⁶: a) longitudinal shock stress, b) shear stress, c) damage-injury metric, and d) shock velocity vs. particle velocity. Compressive strain is measured by the density ratio as $1 - \rho_0/\rho$. Results shown for saline-treated dog lung under uniaxial shock compression.

List of Symbols, Abbreviations, and Acronyms

TERMS:

1-D	one-dimensional
2-D	two-dimensional
3-D	three-dimensional
ARL	Army Research Laboratory
ATBM	Advanced Total Body Model
DEVCOM	US Army Combat Capabilities Development Command
DOP	depth of penetration
FE	finite element
KE	kinetic energy

MATHEMATICAL SYMBOLS:

t	time
D	local damage-injury metric
$\mathbf{F}, F_{ij}$	deformation gradient
$\mathbf{R}, R_{ij}$	Gram rotation matrix (orthogonal transformation)
$\mathbf{U}, U_{ij}$	Laplace stretch tensor (upper triangular)
$\mathbf{X}, X_k$	Cartesian coordinates
ω_D	gradient/rate amplification factor for damage and injury kinetics
$\mathbf{v}, v_k$	velocity

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