UNIVERSITY OF CALIFORNIA SANTA CRUZ

VISUALIZATION TECHNIQUES FOR COMPUTATIONAL MECHANICS

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 in

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by

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Abstract

Visualization Techniques for Computational Mechanics

by

Alisa Gail Neeman

Scientists and engineers use visualization techniques to turn the numerical results from a solid or fluid mechanics simulation into interactive graphics that help them understand the results. This work provides visualization techniques for stress, strain (second-order tensor fields) and stiffness (fourth-order tensor fields). The techniques are applied to data from Geomechanics, a branch of civil engineering focused on predicting how earth-quakes affect soil and infrastructure such as buildings and bridges. The resulting visualizations help illustrate the state of the simulation and facilitate prediction of solids' failure under stress. The main contributions in this work include (i)a decomposition method to reduce fourth-order tensors to second-order which highlight features of interest, (ii) a new visualization technique for second-order tensors, and (iii) an open source visualization application that facilitates finding critical regions of a solid volume and details within those regions.

In loving memory of my father, Dr. Moshe Neeman.

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Chapter 1

Introduction

One unsolved problem for the mechanics of solids and structures is visualizing tensor data. Civil, mechanical, aeronautical, biomedical, material and other branches of engineering dealing with modeling and simulation produce tensor data during design, test, and research. The particular focus and application of this work is visualization for Geomechanics, a branch of civil engineering concerned with the behavior of geomaterials. However, the results are broadly applicable.

To date, the breadth of visualization technique research for solid (non-fluid) mechanics tensor data has been limited. The tensors are non-positive-definite and some features of interest are unique to the domain.Meanwhile, the techniques (formulations, algorithms and implementations) for computational modeling and simulation of materials have advanced at a rapid pace. While the simulation results are now available, the pictures that will help in understanding those results are absent. (Until now, engineers have mainly used a stress-strain curves to illustrate detail or color mapped scalar fields.) Moreover, civil engineering design has evolved in such a way that behavior of critical parts of solids and structures depend on the specific materials and/or components used in an object. Finally, civil engineering materials are loading-history dependent; that is, their behavior is a function of their previous loading history. For example, soils that have been previously compressed will be much stiffer than those not compressed in their loading history. This dimension adds an additional challenge to presenting the most interesting and important parts of the data in a way that is useful and understandable to a wide audience of practicing engineers, researchers, and students.

1.1 Main Contributions

The main work addresses a specific need for the visualization of solids and structures: a representation for the governing equation or constitutive relation. The constitutive relation represents the relationship between applied stress and the resultant strain (deformation) that a material undergoes. The stiffness of the material is described by a fourth-order tensor, and the stress and strain are represented by symmetric secondorder tensors. This thesis makes several contributions that advance visualization of stress, strain, and stiffness tensor fields. First, we found an engineering decomposition of the fourth-order stiffness tensor that allows us to search for the most critical features (modes of softening) and visualize them as second-order tensors. Second, we provide a new glyph-based visualization technique for second-order stress and strain tensors. We present filtering approaches using tensor invariants and other derived features to find critical regions in a stiffness, stress or strain tensor field. Finally, we explore continuous visualization across a volume.

1.2 Auxiliary Artifacts

During the course of the investigation we used the OpenSees earthquake engineering simulator[62]. It was necessary to interface directly with the source code to extract never-before-seen data. I developed an open source visualization application (VEES[57]) that works in tandem with OpenSees. The design of the interface applies principles from the information visualization discipline to the domain of scientific visualization. The beta version has had 4000 downloads from 2006 to 2009 and feedback from the civil engineering research community has been positive.

1.3 Dissertation Organization

This work starts with a short introduction to the tensor notation used (chapter 2) and solid mechanics modeling (chapter 3). This is followed by related work on tensor visualization (chapter 4). Before the chapter on the new decomposition for fourth-order stiffness tensors, there is a short chapter on converting fourth-order tensors to an equivalent second-order representation (chapter 5), which the decomposition requires. The decomposition (chapter 6) and second-order visualization methods (chapter 7) follows, detailing the major visualization contributions in this work. Finally, there are a tutorial and design documentation for VEES (chapter 8).

Chapter 2

Tensor Basics

This chapter explains the mathematical notation used in the dissertation and frequently used mathematical tensor operations as a prelude to domain-specific feature extraction. If the reader is familiar with linear algebra and tensor calculus, this chapter can be read lightly or skipped.

All tensors have an order and dimension, and the components of a tensor are always referenced to a particular basis[11]. Weisstein describes an n^{th} order tensor in m dimensional space as a mathematical object with n indices and m^n components[78]. The order of a tensor refers to the number of rows, columns, stacks, etc. It is also the number of indices. Each index ranges over the number of dimensions of a space[78]. The dimension of a tensor is the number of components in a single row or column (so Cartesian tensors, for example, have dimension 3). A zeroth-order tensor is a scalar and has no indices, a first-order tensor is a vector and has one index, and a second-order tensor can be represented as a square matrix with two indeces. A fourth-order tensor in three dimensions will have 3^4 or 3x3x3x3 components. Tensors of order one or higher have a rank. We use Brannon's definition of rank as the number of linearly independent rows or columns[13].

This work focuses on visualizing 3D second-order tensors (3x3), and analysis with 6D second-order tensors (6x6) and 3D fourth-order tensors (3x3x3x3).

2.1 Einstein Notation

It is much easier to read and think about tensors by using Einstein notation. In Einstein notation subscripts and superscripts are used for each dimension of a tensor (and the order can be deduced from the number of subscripts and superscripts). For example, second-order stress tensors are represented by σ_{ij} where i = 1, 2, 3 and j =1,2,3, and 1,2,3 are orthogonal axes in a Cartesian coordinate system. Second and higher order tensors are shown in bold font where subscripts do not indicate their order.

In Einstein summation, a subscript character repeated in two or more tensors is used to imply tensor entries being summed over. The tensor entries are multiplied together before being added to the sum when there are repeated subscripts and no operator between two tensor operands. Einstein summation is a convenient way to show common tensor operations succinctly.

2.2 Common Operations

Below are some tensor operations and properties important for this thesis. Hopefully they will assist the reader with the notation in later chapters.

2.2.1 Inner Product

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Here we use inner product (or dot product) as a primary example of Einstein summation. Given vectors v_i and w_i , the inner product is calculated as:

$$c = \sum_{i=1}^{n} v_i \cdot w_i = v_1 w_1 + v_2 w_2 + \dots + v_n w_n$$
(2.1)

Using Einstein summation the inner product can be represented more simply

$$c = v_i w_i \tag{2.2}$$

The term single contraction refers to a singly repeated index, which occurs in both inner product and matrix multiplication. We define it more specifically: the order of the result is one less than the highest order operand. This excludes matrix multiplication. Below is an example:

$$w_i = \sigma_{ij} \, v_j \tag{2.3}$$

This can be implemented in a doubly nested for loop.

```
for( i = 0; i < dim; i++) {
   for (j = 0; j < dim; j++) {
      w[i] = w[i] + sigma[i][j]*v[j];
   }
}</pre>
```

2.2.2 Scalar Multiplication

When multiplying a scalar times a vector or tensor, each component is multiplied by the scalar. For this case we omit subscripts. For example, if we have a vector \mathbf{v} , $[v_1 \ v_2 \ v_3]$ and scalar c, the scalar product $c\mathbf{v}$ is

$$c v_i = [cv_1 \ cv_2 \ cv_3]$$
 (2.4)

2.2.3 Matrix Multiplication

Matrix multiplication yields a new matrix, as follows:

$$C_{ik} = A_{ij} B_{jk} \tag{2.5}$$

We represent matrix multiplication without subscripts:

$$C = A B \tag{2.6}$$

This convention is for brevity and to contrast with other operations. In matrix multiplication, the multiplicands and result all have the same order, whereas the result of tensor contraction has a lower order.

2.2.4 Double Contraction

Below a fourth-order tensor is contracted with a second-order tensor to produce a second order tensor. Double contraction reduces the order of the tensor by two.

$$\sigma_{ij} = E_{ijkl} \,\epsilon_{kl} \tag{2.7}$$

The subscript order assists the reader to know which components are multiplied before

the summation. This can be implemented in a nested for loop.

```
for( i = 0; i < dim; i++) {
  for( j = 0; j < dim; j++ ) {
    for(k = 0; k < dim; k++ ) {
      for (m = 0; m < dim; m++ ) {
         sigma[i][j] = sigma[i][j] + E[i][j][k][l]*epsilon[k][l];
      }
    }
  }
}</pre>
```

2.2.5 Outer Product

Outer product or tensor product takes a tensor of order n and dimension m, and a second tensor of order p and dimension q and creates a new tensor with $(m^n \times q^p)$ components. The order of the new tensor will depend on the choice of layout of the components. For example, with two first-order tensors (i.e., vectors), the resulting second order tensor would be built:

$$\begin{bmatrix} p_1 \\ p_2 \end{bmatrix} \begin{bmatrix} q_1 & q_2 \end{bmatrix} = \begin{bmatrix} p_1q_1 & p_1q_2 \\ p_2q_1 & p_2q_2 \end{bmatrix}$$
(2.8)

More formally, the forms of notation for outer product are

$$p \otimes q = p_i q_j = p q^T \tag{2.9}$$

The superscript T denotes transpose. Outer product is distinguished from inner product by not repeating indices $(i \neq j)$. The outer product of two vectors such as \mathbf{p} and \mathbf{q} is a dyad, which has a rank of one even though it is a second-order matrix with dimension greater than one. It has a single non-zero eigenvalue and its eigenvector is equivalent to the first operand (**p**). In this dissertation, either Einstein summation or the outer product symbol \otimes is used, but \otimes is preferred to distinguish more easily from inner product or matrix multiplication.

2.2.6 Eigen-Decomposition

A second-order tensor ${\bf S}$ can be decomposed into two matrices ${\bf M}$ and ${\bf T}$ such that

$$S = T M T^T, (2.10)$$

where \mathbf{T} is the column ordered matrix of eigenvectors, \mathbf{T}^T is the transpose of \mathbf{T} , and \mathbf{M} is a diagonal matrix. The diagonal components λ_i of \mathbf{M} are the eigenvalues corresponding to the eigenvectors in the columns of T. For each eigenvector \mathbf{t} and corresponding eigenvalue λ ,

$$S_{ij} t_j = \lambda t \tag{2.11}$$

2.3 Properties of Tensors

2.3.1 Symmetry

One key property of tensors that simplifies operations is symmetry. According to Weisstein, an object is symmetric if it is invariant under a symmetry operation. In the case of tensors, the symmetry operation is changing the order of indices[78].

2.3.2 Symmetry of Second-Order Tensors

Second-order symmetric tensors are described mathematically using a 3x3 matrix where the off diagonal components are equal: $S_{ij} = S_{ji}$, for $i \neq j$. The matrix looks thus:

$$S = \begin{bmatrix} S_{11} & S_{12} & S_{13} \\ S_{12} & S_{22} & S_{23} \\ S_{13} & S_{23} & S_{33} \end{bmatrix}$$
(2.12)

In other words $\mathbf{S} = \mathbf{S}^T$, where \mathbf{S}^T is the transpose of \mathbf{S} . If a second-order tensor is symmetric, its eigenvectors will be orthogonal and the eigenvalues will all be real.

2.3.2.1 Separating a Second-Order Tensor Into Symmetric and Antisymmetric Parts

The symmetric part of a second-order tensor can be calculated:

$$sym(S) = \frac{(S+S^T)}{2}$$
 (2.13)

The antisymmetric part, which satisfies $\mathbf{S} = -\mathbf{S}^T$, can be calculated:

$$antisym(S) = \frac{(S - S^T)}{2} \tag{2.14}$$

The tensor \mathbf{S} is the sum of the symmetric part and the antisymmetric part.

2.3.3 Symmetry of Fourth-Order Tensors

Fourth-order tensors may have symmetry either within or across pairs of indices. Major symmetry is across pairs of indices, i.e. $E_{ijkl} = E_{klij}$. Minor symmetry is within major pairs, i.e. $E_{ijkl} = E_{jikl} = E_{ijlk} = E_{jilk}$.

2.3.4 Positive-Definiteness

A matrix \mathbf{A} is positive definite if, and only if, for any non-zero vector \mathbf{x} with the same dimension

$$x^T A x > 0 \tag{2.15}$$

holds [78]. Here x are column vectors.

It is also the case that a matrix is positive definite if its symmetric part has all positive eigenvalues. Equation 2.15 only operates on the symmetric part of the matrix. Consider the equation operating on the antisymmetric part, where B = antisymm(A):

$$x^T B x = x_i x_i b_{ii} + x_i x_j b_{ij} (2.16)$$

where $i \neq j$. For each b_{ij} in the upper triangle of the antisymmetric part of the tensor there is a corresponding $-b_{ji}$ in the lower triangle of the tensor and so all $x_i x_j b_{ij}$ in the sum will cancel out, and all the diagonal components b_{ii} of the antisymmetric part are zeros.

2.3.5 Singularity

A matrix is said to be singular if and only if its determinant is zero[78]. Other characteristics are that the matrix will have at least one zero eigenvalue since the determinant is the product of eigenvalues of the matrix. A singular matrix is not invertible. The inverse of a matrix is denoted with a superscript of -1, e.g. \mathbf{M}^{-1} .

Chapter 3

Continuum Mechanics and Solid Modeling

In this chapter we present the basic concepts of models for materials' constitutive relationships. A constitutive model is a set of equations relating stress to strain and possibly other pertinent quantities[10]. We start with the simplest model (one dimensional elastic) and then explain how more complicated material properties are modeled (anisotropy, non-linear elastic, elastic-plastic) in two dimensions and three dimensions. We neglect thermodynamic effects here.

Prevost and Popescu [63] note that at the macroscopic scale, there is great similarities in behavior of a wide variety of materials. They state:

Paradoxically, despite the large differences in the nature and structure of materials such as metals and alloys, polymers and composites, concretes, soils, there is a great unity displayed in their macroscopic behavior. With different orders of magnitude, terms like elasticity, viscosity, plasticity, hardening, softening, brittleness and ductility can be applied to all these materials. The models in this chapter start with generally applicable models and move toward soil-specific models. Finally, we touch on critical features for soils and solids. The information in the first three sections is derived from Wood [81] and Roylance [65] and later sections from Jeremić [35] and Prevost and Popescu [63].

3.1 Hooke's Law - the Basic Constitutive Equation in 1D

For the one dimensional case, we look at a model for a simple elastic spring. This basic relation is the basis of more complicated and higher dimension models, so



Figure 3.1: Spring response under applied force

it is worth mentioning. All terms in a constitutive relation are constants. Hooke's law summarizes the elastic relationship:

$$F = kx \tag{3.1}$$

Here x is the change in length, the spring's response to the applied force. The spring constant, or stiffness, is represented by k, and F is the applied force. We are interested

in understanding, through visualization, the relationship between applied force and material response.

3.2 Stress and Strain Tensors

Stress is force per unit area, and in 3D it is a second-order symmetric tensor described as follows:

$$\sigma_{ij} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix}$$
(3.2)

The stress tensor is in Cartesian space, so subscripts 1, 2, and 3 correspond to X, Y and Z axes. The diagonal components of the tensor, σ_{ii} , represent normal stresses (The components represent magnitude of stress along Cartesian axes X,Y and Z). The offdiagonal components $\sigma_{ij}, i \neq j$ represent shear stress. The shear components represent stresses along facets orthogonal to the normal stress as shown in figure 3.2. The offdiagonal components are symmetric, i.e. $\sigma_{ij} = \sigma_{ji}$.

Strain (ϵ) is dimensionless change in length, $\frac{\Delta length}{original length}$. The strain tensor components, like stress, are symmetric and represent strain in the same corresponding directions.



Figure 3.2: Stress tensor components.

3.2.1 Two Useful Scalars Describing Stress

Two scalars frequently used in solid modeling are derived from stress components. *Mean stress* is a scalar invariant, calculated by averaging the normal components, i.e.

$$p = \frac{\sigma_{ii}}{3} \tag{3.3}$$

in the case of 3D. It represents volumetric or isotropic stress, such as pressure, that is the same from every direction. Note that in soil literature, mean *effective* stress, p' is calculated. "Effective" refers to total stress minus the effects of pore pressure (from water or air) in the soil.

Deviatoric or distortional stress describes strictly anisotropic forces. These include shear components and differences in force along the normal directions. The stress invariant q quantifying deviatoric stress is calculated:

$$q = \sqrt{\frac{(\sigma_{22} - \sigma_{33})^2 + (\sigma_{33} - \sigma_{11})^2 + (\sigma_{11} - \sigma_{22})^2}{2} + 3(\sigma_{12}^2 + \sigma_{23}^2 + \sigma_{31}^2)}$$
(3.4)

3.3 Two and Three Dimensional Continuum Solids

In order to model the behavior of a surface or volume, their stiffness must be quantified with more than a single constant. Tensors are used, but certain variables help describe the components of the tensor, and symbolize the solid materials' laboratorymeasurable attributes.

3.3.1 Stiffness versus Compliance

By convention, Hooke's Law is written in the form in equation 3.1. However, it can also be written

$$x = \frac{1}{k}F\tag{3.5}$$

The the 2D or 3D tensor representing k is called the stiffness tensor and the tensor representing $\frac{1}{k}$ is called the compliance tensor. The compliance tensor is the inverse of the stiffness tensor.

Analytically, stress is assigned and strain is calculated using the compliance tensor. Numerically, however, strain is assigned and stress is calculated using the stiffness tensor. In this section we look at relationships using the compliance tensor.

3.3.2 Important Solid Material Constants

As with the one dimensional case there are several important constants that help to specify behavior of elastic material. First, there is Young's modulus(E):

$$E = \frac{\frac{F}{A}}{\frac{\Delta l}{l}} \tag{3.6}$$

E represents the amount of elongation a material undergoes in relation to the applied stress. F is force, A is area over which the force is applied, and $\frac{F}{A}$ is stress. The fraction $\frac{\Delta l}{l}$ is change in length divided by length and represents the unitless strain. It is useful to think of a wire in uniaxial tension. A is then the area of the wire's cross section and l is how much it got stretched.

Poisson's ratio helps describe deformation on an axis or plane *orthogonal* to where the length measurement (in equation 3.6) is taken.

$$\nu = \frac{\frac{\Delta d}{d}}{\frac{\Delta l}{l}} \tag{3.7}$$

Here d is diameter. Thinking again of a wire in uniaxial tension, you can imagine the wire getting thinner (d reducing) as it gets stretched; this is the Poisson effect. Like Young's modulus, Poisson's ratio is dimensionless.

Two useful scalars calculated in terms of E and ν are the bulk modulus K and shear modulus G. Bulk modulus describes resistance to isotropic stress, stress which causes a change in volume without a change in shape.

$$K = \frac{E}{3(1-2\nu)} \tag{3.8}$$

You can imagine how a soft ball might respond to pressure (equal force from every direction) by becoming more compact, but keeping its round shape.

Shear modulus G describes the converse case, how a material resists stress that causes a change in shape without change in volume.

$$G = \frac{E}{2(1+\nu)} \tag{3.9}$$

3.3.3 Intuition

A 2D tensor can be used to show a 3D triaxial state of stress, if it describes a uniaxial force on the vertical and a second, radial force around the diameter on the horizontal plane, as shown in figure 3.3.3. We can use the lower dimension tensor because the system it represents is an axis and a plane rather than a basis of three axes.



Figure 3.3: Triaxial Stress.

Wood provides a tensor for the constitutive relationship in terms of Young's modulus and Poisson's ratio[81]:

$$\begin{bmatrix} \delta \epsilon_{axial} \\ \delta \epsilon_{radial} \end{bmatrix} = \frac{1}{E'} \begin{bmatrix} 1 & -2\nu' \\ -\nu' & 1-\nu' \end{bmatrix} \cdot \begin{bmatrix} \delta \sigma'_{axial} \\ \delta \sigma'_{radial} \end{bmatrix}$$
(3.10)

The δ symbols indicate that these are stress and strain *increments*. Note also that this formula is written in terms of the soil's effective stress and related variables are indicated by the prime symbol (').

The off-diagonal components of the compliance matrix are a calculated by multiplying a constant times the fraction $\frac{\nu'}{E'}$, and showing the relationship between the changing length and changing diameter.

3.4 Stiffness As A Tensor

With Hooke's Law, force, deformation and stiffness are all zero order tensors (i.e. scalars). When stress and strain increments are 3x3 symmetric tensors, compliance and stiffness are 3x3x3x3 tensors, with minor symmetry ($C_{ijkl} = C_{jikl} = C_{ijlk} = C_{jilk}$), transforming stress to strain, and vice versa, respectively.

The symmetry in stress and strain force the stiffness and compliance tensor to exhibit minor symmetry. This means stiffness and compliance contain 36 independent components out of 81 total.

The constitutive equation for 3D continuum solids is:

$$\dot{\epsilon}_{ij} = C_{ijkl} \dot{\sigma}_{kl} \tag{3.11}$$

Here, C stands for compliance, and the dot over σ and ϵ denote increments. The constants i, j, k, and l are numbered 1 to 3, corresponding to Cartesian axes X,Y, and Z. It is not assumed that the stress/strain relationship is linear. Therefore the constitutive equation is generalized to express the relationship incrementally[58].

Bower states that these tensors must comply with "material frame indepen-

dence", that is,

the condition that the tensor-valued functions that relate stress to deformation measure must transform correctly under a change of basis and change of origin for the coordinate system[10].

It is easier to understand (and simpler for engineers to make calculations with) stiffness

as a second-order tensor and stress and strain increments as vectors. Because of symmetry, a more compact and efficient representation can be used: 6D vectors for stress and strain increments, and a 6x6 matrix for stiffness or compliance.

Chapter 5 formally describes the orthonormal basis and algorithm for transforming between these two systems, but for clarity we simply use matrices and vectors in this chapter.

3.4.1 Elastic Isotropic Materials

Hooke's Law defines spring-like behavior in solid materials. When force is applied, the spring's length changes, and when it is removed the spring reverts to its original length. Recoverable deformation is referred to as elastic behavior. The simplest material models describe only elastic behavior.

Isotropic materials have equal magnitude responses regardless of the orientation of the solid with respect to the applied force. In other words, the derivative of stress with respect to strain is independent of the orientation of the material[10].

3.4.2 3D case

Here is the constitutive relation for the 3D case according to Bower[10]:

$$\begin{vmatrix} \delta \epsilon_{xx} \\ \delta \epsilon_{yy} \\ \delta \epsilon_{zz} \\ \delta \epsilon_{xy} \\ \delta \epsilon_{xz} \\ \delta \epsilon_{xz} \\ \delta \epsilon_{yz} \end{vmatrix} = \begin{vmatrix} \frac{1}{E} & \frac{-\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & \frac{1}{E} & \frac{-\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & \frac{1}{E} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2G} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2G} & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2G} \end{vmatrix} . \begin{cases} \delta \sigma_{xx} \\ \delta \sigma_{yy} \\ \delta \sigma_{xz} \\ \delta \sigma_{yz} \\ \delta \sigma_{yz} \end{vmatrix}$$
(3.12)

One can see the operation of Young' modulus (E) in conjunction with stress; $\frac{1}{E} \equiv \frac{\Delta l}{lE}$. The ratio $\frac{-\nu}{E}$, highlighted in red, gives us the change in diameter as the length changes. Thus, the diagonal components in the top half of the matrix change length while the off-diagonal components change diameter with respect to length. Because of isotropy, all shear responses are influenced by the same material constant, $\frac{1}{2G}$.

It is clear that in the elastic isotropic material model, if there is a force along X, there is a change in diameter along Y, and vice versa. The proportional constant is the same in both cases due to the isotropy and the result is a fully symmetric compliance matrix; in tensor form we have the additional major symmetry $(C_{ijkl} = C_{klij})$.

3.4.3 Anisotropy

Wood presents a matrix for transverse anisotropy, which typically occurs in a soil sample. He notes, since particles are more likely to move vertically than horizontally (thanks to gravity) the soil's stiffness along these two directions will differ. In the equation below, h stands for horizontal, and v for vertical, and the vertical axis is the z axis.

$$\begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ \epsilon_{xy} \\ \epsilon_{xz} \\ \epsilon_{yz} \end{bmatrix} = \begin{bmatrix} \frac{1}{E_h} & \frac{-\nu_{hh}}{E_h} & \frac{-\nu_{vh}}{E_v} & 0 & 0 & 0 \\ \frac{-\nu_{hh}}{E_h} & \frac{1}{E_h} & \frac{-\nu_{vh}}{E_v} & 0 & 0 & 0 \\ \frac{-\nu_{vh}}{E_v} & \frac{-\nu_{vh}}{E_v} & \frac{1}{E_v} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{2(1+\nu_{hh})}{E_h} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2G_{vh}} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2G_{vh}} \end{bmatrix} \cdot \begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{xy} \\ \sigma_{xz} \\ \sigma_{yz} \end{bmatrix}$$
(3.13)

However, we note that for the *elastic* materials used in Geomechanics, major *and* minor symmetries are retained, despite anisotropy.

3.5 Elasto-plasticity

According to Prevost and Popescu [63], elastic-plastic models are the most promising models for soil. In an elastic-plastic model, with sufficient stress, a material will reach a yield point and have permanent, non-recoverable plastic deformation. The original Hooke's Law (equation 3.1) only describes the elastic, recoverable behavior; the spring returns to its original length when the force is removed.

An elastic-plastic material model needs more descriptive properties. Following Wood [81], the model must include the following:

1. Elastic properties
- 2. Yield Function and Yield Surface
- 3. Plastic Potential or Plastic Flow
- 4. Hardening Rule

The elastic properties are simply a fourth-order symmetric tensor such as those described in equations 3.12 and 3.13. The modeler may simply ask for a set of constants such as Young's modulus and Poisson's ratio and complete the tensor for the user.

A yield function is used to delineate the type of stresses that cause only elastic deformation versus elastic plus permanent, plastic deformation. For example, the Von Mises yield function is:

$$(\lambda_2 - \lambda_3)^2 + (\lambda_3 - \lambda_1)^2 + (\lambda_1 - \lambda_2)^2 = 8c^2$$
(3.14)

Here, λ_i are the eigenvalues, or principal stresses, and 2c is the *yield stress* in uniaxial tension [81]. Either tension, deviatoric stress, or some combination of these can cause a material of this type to yield and deform plastically. Von Mises materials do not yield under isotropic compression or tension (three equal eigenvalues).

Given a space spanned by principal stresses λ_1 , λ_2 , λ_3 , a yield surface forms where a combination of stress eigenvalues signals that a material begins to deform plastically, causing permanent deformation. It is the zero isosurface of the yield function (the contour where the function's value is zero). If plotted in 3D, the function forms a convex surface. In the example given by equation 3.14, the shape is a cylinder, as shown in figure 3.4.



Figure 3.4: Von Mises yield surface in stress space.

More complex material models may have multiple nested yield surfaces, which adds to the complexity of calculating the elastic-plastic stiffness tensor.

The plastic potential, like the yield function, is a function in stress space. Its gradient describes the direction in which the material will flow once it yields.

According to Wood, the hardening rule (or evolution law) changes the size and/or shape of the yield surface (i.e., the criteria for yielding) and magnitude of plastic deformation. Jeremić notes that it can also change the plastic flow directions. The derivative of the yield surface and the derivative of the plastic potential are used to calculate the elastic-plastic stiffness when the yield stress is exceeded.

The hardening rule may be linear or non-linear. It may range from a simple scalar (for isotropic changes) to a fourth order tensor (for anisotropic changes) [35]. The evolution law facilitates modeling behavior like soil becoming stiffer under compression or less stiff under shear, and changes in stiffness under cyclic loading and unloading as experienced during an earthquake.

3.5.1 Nonlinear Elastic Models

Nonlinear elastic models do not have a formal yield surface or plastic potential. Instead, hardening and softening are controlled by functions that change the compliance matrix entries depending on the state of stress. The application of elastic nonlinear models is limited. Prevost and Popescu [63] state:

Although, experience has shown that simple nonlinear elastic stress-strain models like the hyperbolic model are not capable of modeling fundamental aspects of real soil behavior, they still remain popular in practice.

As such, a time-varying visualization technique for stiffness of these models would be particularly critical but very difficult.

Chapter 4

Related Work

Higher order tensor visualization has the least amount of completed work of any branches of scientific visualization. It carries general issues for visualization, for instance, in a 3D field, there is often occlusion, where features may be hidden behind other displayed objects. There are also tradeoffs between high detail and showing the global state of a field.

However, the main challenge for visualization of tensors is to be able to show the domain features in an understandable way. The large number of components describing a tensor must be distilled into color and shape and displayed on a 2D screen.

Cross-applicability of tensor visualization techniques across science and engineering domains is difficult. Domain features of interest often can limit transferability. For example, tensors from different domains exhibit mathematical features that limit cross-applicability, such as varying kinds of symmetry, positive-definiteness (or lack) and varying order. Table 4.1 summarizes the major domains, their tensors' meaning, and

Meaning	Order	Features		
Stress	Second	Symmetric		
Velocity Gradient	Second	Nonsymmetric		
H_2O molecule diffusion	Second or Fourth	Symmetric,		
		Positive-Definite		
Moment at fracture	Second	Symmetric		
Stress	Second	Symmetric		
Strain	Second	Symmetric		
Stiffness	Fourth	Non-Major-		
		Symmetric,		
		Positive-Semi		
		or Non-Positive-		
		Definite		
	Meaning Stress Velocity Gradient H_2O molecule diffusion Moment at fracture Stress Strain Stiffness	MeaningOrderStressSecondVelocity GradientSecondH2O molecule diffusionSecond or FourthMoment at fractureSecondStressSecondStrainSecondStiffnessFourth		

Table 4.1: Scientific and engineering domains' tensors and their features.

their mathematical features. As tensor visualization techniques have developed, crosspollination of ideas rather than direct transfer to new domains has often occurred. This chapter presents a survey of tensor visualization techniques, with a focus on discovering what works well for solid mechanics tensor data.

The chapter is organized with a section for second-order tensors and one for fourth-order tensors. In the section on second-order tensors, streamline techniques are discussed first, followed by glyphs. In the fourth-order section, the order is reversed since the streamline features are based on the meaning of a specific glyph which is introduced first. DT-MRI is the acronym for Diffusion Tensor Magnetic Resonance Imaging. It is used in medicine to determine the health of neurons in the brain and heart muscle tissue.

4.1 Vector Fields

Continuous tensor visualization techniques (integrating over a plane or volume) grew out of vector field visualization techniques which we discuss first.

4.1.1 Streamlines

Streamlines are a visualization technique originally used for a static vector field such as a single time step for air or wind flow. Streamlines are tangent to the flow. The idea is analogous to placing smoke emitting flares in the wind field and observing the direction of the smoke trails (streak lines). To visualize this, seed points are placed in the vector field where they are integrated along the direction of the vector. The number and placement of seed points is a key issue[76, 42, 77, 55, 69, 70, 82]. In 2D, the visualization can become overly cluttered and in 3D, features may be occluded.

One common method for integration method used for streamlines is fourthorder Runge-Kutta (RK4). Runge-Kutta is known for its stability. One needs an integration step size h for time increment t, velocity function V(t,p) and an initial velocity and position $V(t_0), p_0$. "Time" is incremented by:

$$t_{n+1} = t_n + h (4.1)$$

The step p_{n+1} is the RK4 approximation of $p(t_n + 1)$, and p_{n+1} is calculated

$$p_{n+1} = p_n + \frac{1}{6}h\left(k_1 + 2k_2 + 2k_3 + k_4\right) \tag{4.2}$$

where

$$k_1 = V(t_n, p_n) \tag{4.3}$$

$$k_2 = V(t_n + \frac{1}{2}h, p_n + \frac{1}{2}hk_1)$$
(4.4)

$$k_3 = V(t_n + \frac{1}{2}h, p_n + \frac{1}{2}hk_2)$$
(4.5)

$$k_4 = V(t_n + h, p_n + hk_3) \tag{4.6}$$

A variation on streamline visualization is Line Integral Convolution (LIC)[14]. A streamline is calculated for each point in the field. Additionally, a noise texture is generated with the same dimensions as the field. The weighted average of noise textures along a point's streamline determines the shade of the point.

4.1.2 Flow Topology of Vector Fields

Helman and Hesselink felt there was a need to automate the generation of streamlines in vector flow fields. They promulgated the idea of flow topology, with curves or surfaces that divide the flow into separate regions. A key feature is critical points. A critical point is a location where the magnitude of the vector is zero. Helman and Hesselink defined the vector field's topology by taking the Jacobian of the vector field at each point. (Note that the Jacobian is not necessarily symmetric.) Topological features could be categorized as repelling or attracting foci, saddle points, centers of revolving circles of fluid, and repelling or attracting nodes, as shown in figure 4.1. The categorization was based on whether the Jacobian tensor had real or imaginary eigenvalues and the real eigenvalues' signs[27].



Figure 4.1: Critical point classification in a 2D flow field. R: real eigenvalue. I: Imaginary eigenvalue. Image source: [26].

4.2 Second-Order Tensor Fields

The two main types of visualization techniques for second-order tensor fields are hyperstreamlines and glyphs.

4.2.1 Hyperstreamlines

For 2D second-order symmetric tensor fields, Dickinson proposed the idea of tensor lines[18]. The tensor field was preprocessed by eigen-decomposition. The eigenvectors are categorized as major, medium, and minor, where the major eigenvector has the largest eigenvalue, and minor, the smallest. For positive-definite tensors, they are automatically sorted by largest absolute value). Either major, medium or minor eigenvector is selected to be a vector field and streamlines can be traced in the field. In the case of isotropic tensors, (all equal eigenvalues), two issues arise. First, any set of orthogonal vectors can be a set of eigenvectors for the tensor. Second, the ordering of major, medium and minor eigenvectors will be random. In this case, the tensor line may experience sudden changes in direction.

Delmarcelle and Hesselink proposed the idea of hyperstreamlines for 3D tensor fields, where the other two eigenvalues would set the shape, diameter and color[16, 17] of the tensor lines.



Figure 4.2: Hyperstreamlines. Figure source: [16]

4.2.1.1 Topology of Second-Order Tensor Fields

Like vector flow fields, second-order continuous tensor fields have a topology. According to Delmarcelle and Hesselink, the topology is found in the eigenvector fields. Analogous to vector field critical points are the tensor field's degenerate points. These points are defined as locations where there are two equal eigenvalues[17], and the criterion can therefore be applied to 2D or 3D fields. The most elementary singularities in 2D tensor fields are trisectors and wedges, which are composed of of parabolic and hyperbolic sectors. Merging two such degenerate points form the singularities shown in figure 4.1.

The remainder of the topology of tensor fields are separatrices. These boundary curves separate parabolic and hyperbolic sectors in the neighborhood of degenerate points, and connect them[17].

Zheng and Pang discovered that in 3D tensor fields, stable degenerate features form lines[83]. Moreover, Zheng et al found that the 3D degenerate lines are connected



Figure 4.3: Double degenerate lines in a tensor field. Figure source: [83]

by separating surfaces [85].

4.2.1.2 Hyperstreamlines and DT-MRI Data

Hyperstreamlines have also been applied to the second-order symmetric, positivedefinite tensor fields of DT-MRI data. Diffusion Tensor Magnetic Resonance Imaging (DT-MRI) describes diffusion of water molecules through tissue. According to Kindlmann and Weinstein, the key feature of interest is the anisotropic motion of water molecules [45]. They note that with brain scans, doctors wish to visualize white matter, the fibrous structure which connects major regions of the brain. Westin, et al. decomposed MRI diffusion tensors and correlated *linear anisotropy* with the major white matter tracts [79]. The fields represent water molecule diffusion within cells such as muscle fibers and nerve axons. Basser, et al. claimed that the normalized eigenvector associated with the largest eigenvalue lies parallel to nerve fiber tracts[5]. Thus, it is clear that a hyperstreamline representation will give a line-like representation of nerve pathways. However, more complex configurations of fibers (crossings, kissings, T and Y junctions) cannot be distinguished by second-order tensors, partly because the resolution of this data type is not high enough[32].

Scheuermann, et al., tested hyperstreamlines on 3D fields of symmetric stress tensors from solid mechanics[66]. While the results looked promising for simple point loads in elastic materials, the forces were very difficult to interpret in more realistic simulations. Here, the features were tension (positive eigenvalues) and zero determinant (at least one zero eigenvalue), and while it was possible to identify regions of interest, the behavior in those regions was difficult to identify. Jeremic, et al. followed on by exploring the use of hyperstreamsurfaces [38]. While these were more powerful, they required separate visuals for each of the three principal stresses, as hyperstreamlines did, and fell short of providing a visualization that could show all key features. Hashash, et al. also used hyperstreamlines to show loading history for multiple time steps and the stresses experienced at each step. They found it useful for comparing different material models' responses to stress. However, they were unable to identify the signs of the principal stress components (eigenvalues). Further, they were unable to identify where a " K_0 state of stress" might exist[25].

However, simple tensor lines were later successfully used for 2D stress tensors from solid mechanics[80]. Wilson and Brannon, focused on the domain-specific feature of shear in crack propagation. The goal was to find abrupt changes of direction in shear forces. Instead of following the eigenvectors, they used the directions of maximum shear which was simply a 45° rotation of the eigenvectors. The background was colored by magnitude of deviatoric component of stress to emphasize regions of high shear.

4.2.2 Glyphs

Another way of visualizing second-order tensors is with glyphs that are placed at discrete locations in the field, or are used to show detail at a single point. A glyph is a graphical icon that uses color and shape to illustrate features of the object it represents.

4.2.2.1 Hedgehog Glyphs

The simplest stress glyph is the hedgehog glyph. The glyph is composed of lines for each eigenvector. The idea is similar to hyperstreamlines, but is non-continuous. In the case of solid mechanics, the lines represent the orientation of principal stresses. Jeremić et al. found hedgehogs inadequate for understanding the contents of a 3D stress tensor field[37].



Figure 4.4: Hedgehog glyphs in a tensor field resulting from a double point load applied to a volume. Red represents tension, and green, compression. Figure source: [37]

4.2.2.2 DT-MRI Glyphs

An important difference between the diffusion tensors and the solid mechanics stress tensors is that the diffusion tensors are positive definite with positive eigenvalues.

A diffusion tensor is classified based on eigenvalues λ_1 , λ_2 and λ_3 , It is isotropic where $\lambda_1 \simeq \lambda_2 \simeq \lambda_3$, planar anisotropic where $\lambda_1 \simeq \lambda_2 \ge \lambda_3$, or linear anisotropic where $\lambda_1 \ge \lambda_2 \simeq \lambda_3$. The degree of each case is determined as follows:

$$\frac{\lambda_1 - \lambda_2}{\lambda_1 + \lambda_2 + \lambda_3} \qquad \frac{2(\lambda_2 - \lambda_3)}{\lambda_1 + \lambda_2 + \lambda_3} \qquad \frac{3\lambda_3}{\lambda_1 + \lambda_2 + \lambda_3}$$

(linear case) (planar case) (isotropic case) The linear case represents fiber tracts, such as neurons in brain tissue, as described in section 4.2.1.2. Superquadric glyphs have been developed to illustrate continuous gradations between these three categories [49, 44] in a barycentric shape space as shown in figure 4.5. The spherical glyph at (a) illustrates isotropy, (b) illustrates planar anisotropy, and (c) illustrates linear anisotropy. Superquadrics' other advantage of the that they give information about the orientation of the eigenvectors in addition to the type of



Figure 4.5: Superquadric tensor glyphs. Figure source: [44]

anisotropy. However, they are not fully adequate to illustrate stress since they are limited to positive-definite tensors. Several key stress features for solid mechanics, namely shear, triaxial compression and triaxial extension, have both negative and positive eigenvalues.

4.2.2.3 Solid Mechanics Glyphs

A recent study by Hashash et al. [25] evaluated several glyphs in their ability to show stress, strain, and solids' stress-strain response.

Among the glyphs in the study were:

- Lamé stress ellipsoid which was a glyph where its three axes were defined by the absolute value of the magnitudes of the principal stresses.
- Haber glyph which consisted of a cylindrical rod through an elliptical disk. The half length of the rod represented the magnitude of the major principal stress, while the shape of the disk was controlled by the magnitudes of the median and

minor stresses.

- Cauchy's stress quadric glyph which used the tensor components in a quadric surface equation such that the glyph was oriented in the principal directions
- Reynolds stress glyph which was defined such that the distance from the origin of the glyph to any point on its surface is the magnitude of normal stress in that direction



Figure 4.6: Reynolds Glyph for stress tensor with eigenvalues (-0.816, 0.408,0.408). Eigenvectors coincide with Cartesian Axes. Red is X, green is Y and blue is Z.

The authors additionally presented the HWY glyph which was a variation on the Reynolds glyph designed to illustrate shear[25].

The scalar for creating the quadric surface was the square root of the difference of the square of a stress vector on the selected plane and the square of the Reynolds scalar (representing the normal stress on that plane). Table 4.2.2.3 provides the formulas for the quadric glyphs described. Hashash et al. noted different shortcomings with each type of glyph. First, they note Lamé and Reynolds could not show principal directions for nearly isotropic stress. However, with isotropic stress, a single eigenvalue spans the entire space, and the choice of orthogonal eigenvectors (and the principal stresses they



Figure 4.7: HWY glyph for illustrating shear stress, eigenvalues listed in illustration. Image source:[25].



Figure 4.8: Lamé stress ellipsoids for single point load applied on top center of volume (generated with VTK[67]).

represent) is arbitrary.

A serious drawback for the Lamé glyph is that it does not differentiate positive principal stresses from negative. For instance, pure shear, a frequent cause of a solid failure during an earthquake, has a signature of two eigenvalues equal in magnitude but with opposite signs. The Lamé glyph would not help to identify pure shear.

Hashash argued that the Cauchy stress glyph does not have an intuitive shape since,

Name	Formula
Lamé	$\frac{(x_1)^2}{(\lambda_1)^2} + \frac{(x_2)^2}{(\lambda_2)^2} + \frac{(x_3)^2}{(\lambda_3)^2} = 1$
Haber	see description (non-quadric)
Cauchy	$\sigma_{ij}n_in_j = \pm k^2$
Reynolds	$c = \sigma_{ij} n_i n_j$
HWY	$\sigma_{Shear} = \sqrt{(\sigma_{ij}n_j)(\sigma_{ij}n_j) - (\sigma_{ij}n_in_j)^2}$

Table 4.2: Glyph types presented by Hashash et al. [25]. x_i :variables along the principal axes, λ_i : eigenvalues, σ_{ij} :stress tensor components, k:selected constant, and n_i : vector from center to surface of a unit sphere.

"magnitude of the normal stress/strain is inversely proportional to the square of the size" [25]

The appearance of the Cauchy stress glyph is the inverse of a Reynolds glyph. Along the eigenvector with the smallest eigenvalue, the distance from the center of the glyph to the surface is largest. This makes it difficult to interpret the state of stress.

Haber glyphs are ambiguous distinguishing between horizontal and vertical stresses in the case of two identical eigenvalues, and the HWY glyph does not show orientation of shear [25].

4.2.3 Seismology Glyphs

Seismologists use a moment tensor M_{ij} to provide a general representation of a seismic source [19]. Seismic moment tensors are a variation of stress tensor for an elastic substance, similar to stress tensors for Geomechanics. However, they differ in a couple of very important ways. Seismic moment tensors (or acoustic emission moment tensors) are created from a measured event such as an earthquake or cracking solid. Sound waves are emitted at the event and can be measured. Thus, moment tensors represent a strictly elastodynamic source [43]. Second, in Geomechanics, a stress tensor relates to forces applied on the exterior surface of a volume. Moment tensors instead relate to forces that cause displacement across an surface, where the surface represents a buried fault [2].

Seismology "beachball" glyphs provide two kinds of information: (1) the type of fracture mechanism, and (2) the orientation.

The first step in classifying how a solid fails is eigen-decomposition. A diagonalized moment tensor can be further decomposed into isotropic and deviatoric components. A purely isotropic tensor is characterized by three equal eigenvalues. The isotropy in a moment tensor represents a change in volume. Pure isotropy in a moment tensor is comparable to an ideal explosion (positive eigenvalues) or implosion (negative eigenvalues) [20]. The deviatoric component is the remainder of the original matrix after the isotropic component has been removed.

Below is the mathematical notation for the isotropic and deviatoric components of matrix M, where the trace (tr) is the sum of the diagonal elements and m_i^* is $m_{ii} - tr(M)/3$. Note that the convention in this field differs from that of DT-MRI tensors.

$$M = \begin{bmatrix} \frac{tr(M)}{3} & 0 & 0\\ 0 & \frac{tr(M)}{3} & 0\\ 0 & 0 & \frac{tr(M)}{3} \end{bmatrix} + \begin{bmatrix} m_1^* & 0 & 0\\ 0 & m_2^* & 0\\ 0 & 0 & m_3^* \end{bmatrix}$$
(4.7)

Moment tensor elements represent dipoles. A dipole is composed of two equal and opposite vectors laying along an axis orthogonal to both of them. The physical meaning is the direction and angle of earth movement along opposite sides of a fault. According to Dreger *double couple* (DC) consists of two linear vector dipoles of equal magnitude but opposite sign, resolving shear motion on faults oriented 45 degrees to the principal eigenvectors of M_{ij} [19]. This is the same definition of shear used in solid mechanics with stress tensors.

Compensated linear vector dipole (CLVD) refers to when "a change in volume is compensated by particle motion in the plane parallel to the largest stress" [20]. This may be a mechanism for deep earthquakes [46]. CLVD is modeled by eigenvalues proportional to -2, 1, 1, reflecting particle motion. The same eigenvalue signature represents triaxial tension in stress tensors for solid mechanics.



Figure 4.9: Failure modes for moment tensors, p-wave amplitude, and representative beachball glyphs. Note that positive wave amplitudes are compressional, and negative are dilational. Figure source: [20].

Figure 4.9 shows the failure mechanisms associated with pure isotropy, uniaxial tension, DC, and CLVD. For the DC types, the possible shear planes are at the division between positive and negative amplitudes, and the color contrast on the beach balls resolve in sharp lines to emphasize their orientation. (The principal stresses, by implication, are 45° off from them.) Clutter is not a problem for these glyphs since just a few are sprinkled in each neighborhood of an earthquake epicenter or solid fracture.

4.3 Fourth-Order Tensors

Ellipsoidal glyphs have long been used to represent second-order symmetric tensors with applications in engineering. The main glyph technique for visualizing fourth-order tensors is an extension of the Reynolds stress glyph. The formula for a point on the surface of the fourth-order Reynolds glyph is

$$c = E_{ijkl} n_i n_j n_k n_l \tag{4.8}$$

Color is used to show the magnitude of the vector from the origin to the surface points. We extend the color scheme to cover both negative and positive values of vector length since shape alone is ambiguous.

Kriz et al. also used a fourth-order Reynolds glyph representation for materials [48]. The representation came from Christoffel's equation for waves propagating in anisotropic media.

$$[C_{ijk\ell}\nu_i\nu_j - \rho v^2 \delta_{k\ell}]p_k = 0 \tag{4.9}$$

Here, $C_{ijk\ell}$ are major and minor symmetric stiffness tensor components, ν_i are components of the wave direction vectors, v is the wave speed, ρ is density, and p_k is the particle displacement direction cosine (i.e. the eigenvector). In this formulation, there is a direct mapping from ν to eigenvectors and from ρv^2 to eigenvalues. The shape of the glyph is mapped to wave velocity magnitude or the eigenvalues, while the color on the glyph is mapped to vibration direction or eigenvectors.

In a recent paper, Basser and Pajevic [6] applied eigen-decomposition to a fourth-order symmetric covariance tensor for use in DT-MRI. The resulting secondorder eigentensors and their eigenvalues were used to represent and visualize variability. Basser and Pajevic visualized the second-order eigentensors and fourth-order covariance tensors as Reynolds glyphs. While the decomposition was applied to fully symmetric positive definite covariance tensors, it motivated our approach for visualizing nonsymmetric fourth-order stiffness tensors.

4.3.1 HOT-lines

Schutz and Seidel noted that second-order tensors have proved inadequate for tracking neuronal fibers in the case of crossings, kissings, fanning or bending fibers in MRI tensor data[68]. High angular resolution techniques have led to a fourth-order (and theoretically, higher) representation which is now used to resolve such cases.

In HOT-lines, Hlawitschka and Scheuermann [32] used spherical harmonics to compute fourth-order Reynolds glyphs more efficiently. Their method could be applied to fully symmetric tensors of even order on a regular grid, and particularly to fourthorder diffusion tensors from DT-MRI. Equation 4.8 is equivalent to the set of functions of the truncated Laplace's series of spherical harmonics. The spherical harmonics helped detect global maxima on the glyph's surface, which represented directions for tracking fibers in DT-MRI [32]. Although spherical harmonics could also be used to detect minima, it is not clear that it would be meaningful in detecting loss of stiffness. Also, fourth-order stiffness tensors are not fully symmetric, so this technique could not be applied.

Schutz and Seidel noted that the local maxima method underestimates the orientation of fiber tracts by 10°, or ignores non-orthogonal peaks[68]. Their approach was to decompose the high order tensor into an (optional) isotropic part, several rankone high order terms representing peaks, and a small residual representing noise. The isotropic portion represents the ambient part of the diffusion.

Peaks are the set of symmetric rank-one approximations of high order tensors, and represent fiber orientations. The peaks are essentially a scalar multiplied by the outer product of a series of unit length vectors. A narrow peak's sharpness grows with number of vectors in outer product part. (For a fourth-order tensor, there will be four vectors).

Schutz and Seidel's algorithm was iterative. Initially, everything was residual noise in a Q-Ball representation[75], which is an orientation distribution function (ODF). Isotropy was found by computing the mean of homogeneous form of the ODF (using spherical harmonics) and multiplying it by the identity tensor. From the residual of the ODF, each rank-one term was optimized. The Gradient Descent technique was used to find rank-one peaks. A peak was accepted if it significantly reduced the residual norm.

Neither of these streamline techniques seems applicable to fourth-order stiffness

tensors. Maxima on the fourth-order Reynolds glyph do not tell us where stiffness has been reduced, and a rank-one, first-order tensor (i.e., a vector) does not appear sufficient to tell us the mode of stress the solid is vulnerable to.

Chapter 5

Unrolling Tensors To Matrices

A major treatise of this thesis is that tensor decomposition can lead to a reduced number of components for visualization as well as helping to find the most significant data. However, numerical methods do not exist for decomposing fourth-order tensors into eigenvectors and eigenvalues, singular values, or polar stretch plus rotation. Numerical methods for these decompositions only exist for second-order tensors, i.e., matrices. Therefore, a method is needed to unroll a 3x3x3x3 tensor into a 9x9 matrix, establishing the transfer of component locations and the new basis. Additionally, 3x3 tensors must be unrolled into vectors in the same basis to be able to express the full stress-strain constitutive relation.

The most unrolling is the matrix of Mandel components[54]. This unrolling has the advantage of an orthonormal basis. In addition, in the case of minor symmetry in the original 3x3x3x3 tensor ($E_{ijkl} = E_{jikl} = E_{ijlk} = E_{jilk}$), it can be expressed as a 6x6 matrix. Recently, this unrolling has been defined more formally [34], [28], [74]. The Mandel[54] mapping from the fourth-order stiffness to an equivalent 6x6 matrix is shown in equation 5.2, and the mapping from a 3x3 stress or strain tensor to a 6D vector is shown in equation 5.3.

5.1 Basis

The orthonormal basis for the 9x9 matrix is composed with outer products of orthonormal vectors spanning 3D space:

$$e_1 \equiv (1, 0, 0)$$

 $e_2 \equiv (0, 1, 0)$
 $e_3 \equiv (0, 0, 1)$

Tarantola lists the basis components B of the 9x9 matrix as three diagonal elements,

$$B_1 \equiv e_1 \otimes e_1$$
$$B_2 \equiv e_2 \otimes e_2$$
$$B_3 \equiv e_3 \otimes e_3$$

three symmetric elements

$$B_4 \equiv \frac{1}{\sqrt{2}} (e_1 \otimes e_2 + e_2 \otimes e_1)$$
$$B_5 \equiv \frac{1}{\sqrt{2}} (e_2 \otimes e_3 + e_3 \otimes e_2)$$
$$B_6 \equiv \frac{1}{\sqrt{2}} (e_3 \otimes e_1 + e_1 \otimes e_3)$$

and three antisymmetric elements:

$$B_7 \equiv \frac{1}{\sqrt{2}} (e_1 \otimes e_2 - e_2 \otimes e_1)$$
$$B_8 \equiv \frac{1}{\sqrt{2}} (e_2 \otimes e_3 - e_3 \otimes e_2)$$
$$B_9 \equiv \frac{1}{\sqrt{2}} (e_3 \otimes e_1 - e_1 \otimes e_3)$$

Here, \otimes denotes outer product, so, for example, B_4 is a 3x3 matrix with $\frac{1}{\sqrt{2}}$ in the (1,2) and (2,1) components and zeroes for the rest.

5.2 Matrix and Vector Representation

Following Tarantola, the 9x9 matrix representing the fourth-order tensor E can formulated by unrolling each 3x3 submatrix first into a vector. Then one can compose

Matrix	(1,1)	(2,2)	(3,3)	(1,2)	(2,3)	(3,1)	(2,1)	(3,2)	(1,3)
Vector	1	2	3	4	5	6	7	8	9

Table 5.1: Indices for one unrolling from a 3x3 tensor to a vector.

a 9x9 matrix T with its (1,1) component mapping to the (1,1,1,1) entry of E_{ijkl} and so on.

T has nine quadrants of 3x3 components.

$$\begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{bmatrix}$$
(5.1)

The components for each quadrant, in the new basis, are calculated:

$$T_{11} \equiv E_{ijkl}$$
$$T_{12} \equiv \frac{1}{\sqrt{2}} (E_{ijkl} + E_{ijlk})$$
$$T_{13} \equiv \frac{1}{\sqrt{2}} (E_{ijkl} - E_{ijlk})$$
$$T_{21} \equiv \frac{1}{\sqrt{2}} (E_{ijkl} + E_{jikl})$$
$$T_{31} \equiv \frac{1}{\sqrt{2}} (E_{ijkl} - E_{jikl})$$

$$T_{22} \equiv \frac{1}{2} (E_{ijkl} + E_{ijlk} + E_{jikl} + E_{jilk})$$
$$T_{23} \equiv \frac{1}{2} (E_{ijkl} - E_{ijlk} + E_{jikl} - E_{jilk})$$
$$T_{32} \equiv \frac{1}{2} (E_{ijkl} + E_{ijlk} - E_{jikl} - E_{jilk})$$
$$T_{33} \equiv \frac{1}{2} (E_{ijkl} - E_{ijlk} - E_{jikl} + E_{jilk})$$

Stiffness tensors are constrained to exhibit minor symmetry $(E_{ijkl} = E_{jikl} = E_{ijlk} = E_{jilk})$ so it is clear quadrants $T_{13}, T_{31}, T_{23}, T_{32}$ and T_{33} contain all zero entries and can be omitted in the second-order representation.

The minor symmetry also enables a simpler form of the transition to a 6x6 matrix. (These are the Mandel components[54]).

Given a 3x3x3x3 tensor E_{ijkl} with indices E_{1111} through E_{3333} , an equivalent 6x6 matrix M is made by substituting entries from E_{ijkl} and multiplying by the appropriate constants:

$$M = \begin{pmatrix} E_{1111} & E_{1122} & E_{1133} & \sqrt{2}E_{1112} & \sqrt{2}E_{1123} & \sqrt{2}E_{1131} \\ E_{2211} & E_{2222} & E_{2233} & \sqrt{2}E_{2212} & \sqrt{2}E_{2223} & \sqrt{2}E_{2231} \\ E_{3311} & E_{3322} & E_{3333} & \sqrt{2}E_{3312} & \sqrt{2}E_{3323} & \sqrt{2}E_{3331} \\ \sqrt{2}E_{1211} & \sqrt{2}E_{1222} & \sqrt{2}E_{1233} & 2E_{1212} & 2E_{1223} & 2E_{1231} \\ \sqrt{2}E_{2311} & \sqrt{2}E_{2322} & \sqrt{2}E_{2333} & 2E_{2312} & 2E_{2323} & 2E_{2331} \\ \sqrt{2}E_{3111} & \sqrt{2}E_{3122} & \sqrt{2}E_{3133} & 2E_{3112} & 2E_{3123} & 2E_{3131} \end{pmatrix}$$
(5.2)

A second-order symmetric tensor S such as stress or strain, in the same basis will be the transpose of

$$\left(\begin{array}{cccc} S_{11} & S_{22} & S_{33} & \sqrt{2}S_{12} & \sqrt{2}S_{23} & \sqrt{2}S_{31} \end{array}\right)$$
(5.3)

The transpose makes the form of the constitutive equation for solid mechanics appear as in chapter 3.

Chapter 6

Decomposition of Fourth-Order Stiffness Tensors for Visualization

A major focus of current research in civil, mechanical and other branches of engineering is modeling and simulating behaviors of solids and structures made up of various materials (soils, concrete, steel, etc.). Realistic models of solids allow engineers to design safer machines and structures. The fourth-order 3D stiffness tensor plays a pivotal role in such modeling and simulations. The stiffness tensor represents the relationship between increments of stress and increments of strain. Stiffness changes state during plastic deformation and failure, so visualization is an important tool for providing (1) insight into material behavior and (2) visual verification of a model. Visualization of fourth-order tensors has not been explored in depth previously, as noted in chapter 4. Challenges include (1) the large number of components (3x3x3x3 for 3D), (2) loss of major symmetry and (3) loss of positive definiteness, with possibly zero or negative

Material Behavior	Symmetry	Tensor Properties
elastic	symmetric	positive-definite
elastic-plastic	asymmetry	eigenvalue magnitude reduction,
		nonsingular if hardening
failure, localized	asymmetry	non-positive definite, possibly sin-
		gular

Table 6.1: How a stiffness tensor can change with increasing stress.

eigenvalues.

One goal of this work is to find a decomposition that (a) reduces the number of components to visualize and (b) highlights the most interesting regions of a volume. The term "interesting" is domain dependent, but the decomposition should be general enough to be useful for many branches of engineering that model and simulate solids. We present a decomposition of fourth-order tensors that facilitates their visualization. The method can be applied to many solid mechanics applications, including Geomechanics. It highlights susceptibility to failure, a feature of interest for engineers.

6.1 Stiffness Changes

Solid materials undergo a sequence of changes under increasing loads. In general, increasing loads beyond the elastic limit induce changes in the stiffness tensor described in table 6.1.

6.1.1 Elastic Behavior

In this dissertation, "elastic" is used synonymously with temporary deformation; the deformation reverses on removal of forces. As an example of elastic deformation, imagine a paper clip: it will elastically change shape to hold a small stack of papers, suffering virtually no permanent deformation after the papers are removed. Brannon notes plasticity theories typically presume that there exists some contiguous domain of stress levels for which permanent (non-recoverable) deformation is negligible [58]. The governing equation to be solved is

$$\dot{\sigma}_{ij} = E^e_{ijkl} \dot{\epsilon}_{kl} \tag{6.1}$$

Here, E^e symbolizes elastic stiffness $\dot{\sigma}_{ij}$ symbolizes stress increments and $\dot{\epsilon}_{kl}$ symbolizes strain increments. Elastic stiffness tensors are both major symmetric ($E^e_{ijkl} = E^e_{klij}$) and minor symmetric ($E^e_{ijkl} = E^e_{jikl} = E^e_{ijlk} = E^e_{ijlk}$), as well as positive definite.

6.1.2 Elastic-Plastic Behavior

We use the word "plastic" synonymously with permanent deformation. When a paper clip is deformed by a large amount, only a portion of the deformation is recovered upon removal of the force. As discussed by Brannon [12], this familiar observation is generalized in plasticity theory with the strain increment $\dot{\epsilon}$ as a sum of a recoverable elastic part plus a permanent plastic part. The onset of plastic deformation is extremely important. With permanent deformation, a machine part may need to be repaired or replaced. A building may become unsafe. The soil may no longer be able to support a bridge adequately. The governing equation for elastic-plastic behavior is

$$\dot{\sigma}_{ij} = E^{ep}_{ijkl} \dot{\epsilon}_{kl} \tag{6.2}$$

where E^{ep} symbolizes elastic-plastic stiffness.

Materials modeled as elastic-plastic are characterized by a yield function, $F(\sigma_{ij})$, a function of stress.(See chapter 3 for more details). The yield criterion, which delineates points at which stress causes elastic-plastic deformation versus pure elastic deformation, is defined at

$$F(\sigma_{ij}) = 0 \tag{6.3}$$

The yield surface is the zero isosurface as described by equation 6.3. Stress states causing $F(\sigma_{ij}) < 0$ correspond to elasticity. Stress states causing $F(\sigma_{ij}) \ge 0$ are attainable only via plastic loading[12], a type of loading that causes some permanent deformation.

6.1.3 Hardening and Softening

Classical equations of plasticity theory model the stress increment as a fourthorder elastic-plastic stiffness tensor acting on the total strain increment [12]. The elastic-plastic stiffness tensor's formulation is a function of the elastic stiffness, yield function $F(\sigma_{ij})$, plastic flow function $G(\sigma_{ij})$, and other internal model variables. A "non-hardening" material has a fixed yield surface. Brannon notes that during plastic loading of non-hardening materials, the stress increment is constrained to move tangent to the yield surface, and the elastic-plastic stiffness tensor is a positive-semi-definite rank-one projection operator. It essentially removes the part of the elastic stress increment that points outside the yield surface [58].

For a hardening material, the yield surface can expand outward, as shown in figure 6.1. Then, increasingly higher levels of stress are required to continue plastic loading. In this case, the elastic-plastic stiffness tensor is positive definite and invertible (non-singular).



Figure 6.1: Yield surfaces (meridian plane) with various types of hardening or softening. p: volumetric stress (pressure), q: deviatoric (distortional) stress. Figure source: [35]

For a softening material, the yield surface contracts in the neighborhood of the stress, so diminishing stresses are needed to continue plastic loading Brannon notes that in this case, the elastic-plastic stiffness tensor can become non-positive definite[58]. Depending on the nature of the loading, softening can lead to an instability in the material response that is characterized by an intense localization (increased strain rate in a defined region) of the deformation in narrow bands[73].

6.1.4 Localized Failure

With enough bending force, a paper clip will deform permanently and eventually break. According to early literature, a solid (in this case a clip) is said to "fail locally" when the stiffness tensor is singular. Here, "locally" means that the solid breaks or liquefies at a set of points, or region, inside the domain [53, 61, 64]. Singularity is identified by one or more zero eigenvalues. Later literature identified localized failure at the point of loss of positive definiteness [61]. A primary goal of this visualization work is to filter the field of evolving tangent stiffness tensors to identify regions near or beyond the localization threshold and to visualize the corresponding modes of susceptibility to failure.

6.2 Related Work on Decomposition

In 2007, Basser and Pajevic [6] applied eigen-decomposition to a fourth-order symmetric covariance tensor for feature detection in DT-MRI, producing a set of six second-order eigentensors. The authors also noted that the mathematical underpinnings of these eigentensors came from Lord Kelvin's work to identify modes of deformation in linear elastic solids. Eigentensors have also been used to classify symmetries in anisotropic solids such as crystals[72].

While Basser and Pajevic applied the decomposition to fully symmetric positivedefinite covariance tensors, these ideas motivated our own research with respect to more general fourth-order stiffness tensors. It seemed plausible that the loss of stiffness would cause a significantly lowered eigenvalue, and I posited that the eigentensor associated with this eigenvalue might have some relation to the mode of stress that would cause large deformation.

Maier and Hueckel gave the criterion for a solid breaking (bifurcation or failure) as a singular stiffness tensor[53]. This criterion is significant because a singular stiffness must have at least one zero eigenvalue. Neilsen and Schreyer were the first to use an eigen-decomposition procedure to determine the deformation mode associated with the bifurcation[61]. Their criterion for bifurcation was the loss of positive definiteness, which occurs before singularity. First, they performed a decomposition to obtain the symmetric part of the stiffness,

$$sym(E) = \frac{1}{2}(E + E^T)$$
 (6.4)

since **E** is positive definite if and only if $sym(\mathbf{E})$ is positive definite. Then they followed with eigen-decomposition on the symmetric part of the stiffness tensor. When positive definiteness was lost, they used the eigentensor of the zero eigenvalue of $sym(\mathbf{E})$ as the mode of bifurcation. Note that the eigentensor of $sym(\mathbf{E})$ is not necessarily an eigentensor of **E** itself, unless **E** is symmetric.

6.3 Our Approach

We should be able to detect susceptibility to failure and nature of the stiffness' vulnerability, in terms of stress. In our approach, we perform a polar decomposition on the stiffness, followed by eigen-decomposition on the polar "stretch". The two step decomposition was proposed by Brannon[58]. Polar decomposition is a technique to separate a matrix into two component matrices,

$$E = R S \tag{6.5}$$

where **S** is a pure stretch (symmetric positive-semidefinite matrix), and **R** is a pure rotation (orthonormal matrix) [29, 22, 31, 30, 86, 24]. Polar decomposition is known in plasticity and mechanics literature, but our use of it for analyzing the stiffness tensor is new. Nielsen and Schreyer [61] showed that eigen-decomposition on the symmetric part of the stiffness tensor produced the critical deformation mode at failure. Like Nielsen and Schreyer, we can detect the loss of stiffness when a significantly low eigenvalue occurs. With polar decomposition, however, Brannon posits that the eigentensor associated with a significantly low eigenvalue represents the stress mode that will produce the greatest deformation. The polar decomposition also appears to tell us about the changing flow direction of permanently deforming material.

6.3.1 Method Constraints

Brannon's decomposition recovers facets of the original modelers' composition. However, it also leads to some constraints on the range of models where the method can be applied. Our method can be applied to stiffness tensors exhibiting the following properties:

• Fourth-order tensors with minor symmetry: The method relies on the secondorder tensors (stress and strain increments) being symmetric, which constrains
the fourth-order stiffness tensor to exhibit minor symmetry.

- *Elastic-plastic material models*: Our method is applicable to general elastic-plastic models, and it can also be applied to any material behavior where the stiffness tensor changes as the loading progresses such as pressure sensitive elasticity or damage.
- Small deformation theory: According to Brannon, "Small deformation" refers to problems with only small displacement gradients. This means that the stiffness tensors are cast with respect to the reference configuration such that any changes in stiffness associated with rigid material rotation are eliminated from consideration[58].
- Absence of elastic-plastic coupling: With elastic-plastic coupling, plastic flow can affect the elastic properties [12]. and is an additional source of non-associativity [33].

6.3.2 Method Details

Our decomposition is composed of the following steps:

- Unroll the 3 × 3 × 3 × 3 tensor into a 6 × 6 matrix using Mandel components (See chapter 5 for details). The 81-component stiffness tensor has 36 independent components, preserved in the new basis.
- 2. Perform a polar decomposition on the 6×6 matrix, producing two 6×6 matrices: the *rotation part* and the *stretch part*.

- 3. Perform an eigen-decomposition on the *stretch part* of the polar decomposition, yielding 6 eigenvectors and 6 real eigenvalues.
- 4. Compose an eigenvector into a symmetric 3×3 eigentensor if it has a significantly lower single eigenvalue, reversing the unrolling.
- 5. Visualize the second-order eigentensor with a glyph that shows its structure and also shows significant features such as eigenvalue or mode.

Continuous visualization (integrated across the volume) of the second-order tensor field is also possible.

6.3.2.1 Unrolling

Unrolling from tensor to matrix requires placing the constants in specific matrix entries and multiplying by constants as shown in equation 6.6.

$$M = \begin{pmatrix} E_{1111} & E_{1122} & E_{1133} & \sqrt{2}E_{1112} & \sqrt{2}E_{1123} & \sqrt{2}E_{1131} \\ E_{2211} & E_{2222} & E_{2233} & \sqrt{2}E_{2212} & \sqrt{2}E_{2223} & \sqrt{2}E_{2231} \\ E_{3311} & E_{3322} & E_{3333} & \sqrt{2}E_{3312} & \sqrt{2}E_{3323} & \sqrt{2}E_{3331} \\ \sqrt{2}E_{1211} & \sqrt{2}E_{1222} & \sqrt{2}E_{1233} & 2E_{1212} & 2E_{1223} & 2E_{1231} \\ \sqrt{2}E_{2311} & \sqrt{2}E_{2322} & \sqrt{2}E_{2333} & 2E_{2312} & 2E_{2323} & 2E_{2331} \\ \sqrt{2}E_{3111} & \sqrt{2}E_{3122} & \sqrt{2}E_{3133} & 2E_{3112} & 2E_{3123} & 2E_{3131} \end{pmatrix}$$
(6.6)

This casts the fourth-order tensor in Mandel form[54]. Mandel components provide an orthonormal basis[74]. In addition, they form an isomorphism between the double contraction $(E_{ijkl} \epsilon_{kl})$ and the equivalent single contraction $(M_{ij} \epsilon_j)[6]$. The details of the basis are covered in chapter 5.

6.3.2.2 Polar Stretch and Mode of Vulnerability

Eigen-decomposition is performed on the symmetric stretch matrix \mathbf{S} from the polar decomposition. This can be done using the LAPACK library [3]. We analyze the eigen-decomposition of \mathbf{S} to find the eigenvector associated with its smallest eigenvalue. Then, we convert this first-order eigenvector $V_i, i = 1...6$ to a symmetric second-order eigentensor S_{ij} :

$$S_{ij} = \begin{bmatrix} V_1 & \frac{1}{\sqrt{2}}V_4 & \frac{1}{\sqrt{2}}V_6 \\ \frac{1}{\sqrt{2}}V_4 & V_2 & \frac{1}{\sqrt{2}}V_5 \\ \frac{1}{\sqrt{2}}V_6 & \frac{1}{\sqrt{2}}V_5 & V_3 \end{bmatrix}$$
(6.7)

Equation 6.7 is the inverse of unrolling operation shown in chapter 5 equation 5.3. The initial eigenvalues of a stiffness tensor are based on the bulk modulus and shear modulus of the material, and the initial stiffness matrix is a pure stretch; its rotation component is the identity. With loading forces sufficient to cause plastic deformation, the stiffness may change as described in section 6.1.3, and resistance to certain types of stress increments may be reduced.

A polar decomposition of stiffness matrix \mathbf{E} quantifies this degradation. Loosely, eigenvalues of \mathbf{S} (the "stretches") are larger than their initial values if the material has stiffened. If they are smaller, it has become less stiff. According to Brannon, the corresponding eigentensors of \mathbf{S} represent loading modes [58].

Suppose the stretch eigenvector associated with the smallest eigenvalue is $[0, 0, 0, 1, 0, 0]^T$ (eigenvectors are column vectors). The corresponding normalized stretch eigentensor is:

$$\begin{array}{cccc} 0 & \sqrt{1/2} & 0 \\ \\ \sqrt{1/2} & 0 & 0 \\ \\ 0 & 0 & 0 \end{array}$$

This is a pure shear on the X-Y plane. If the corresponding eigenvalue is 0.75 of its initial value, then the material is 25% less resistant (stiff) to shear on the X-Y plane than it was initially. Selecting the lowest stretch eigenvalue can therefore reveal which regions are suffering significant plastic loading when many different types of materials are used in a simulation. As the stiffness matrix approaches singularity, having a robust computation procedure, as described in section 6.4 is crucial. An eigenvalue approaching zero is considered to be a failure mode for the material.

If **E** is nonsingular and has negative eigenvalues, the physical meaning of the polar decomposition is unclear. Even if a symmetric-antisymmetric decomposition is used instead, its meaning is still unclear. According to Brannon, the occurrence of a negative eigenvalue in the stiffness matrix corresponds to dynamic softening instability, which requires different differential equations of motion[58]. In our visualization, we use a uniquely shaped black glyph to indicate an occurrence of a negative eigenvalue, and interpretation of its mode of vulnerability is not possible.

One issue for visualizing eigentensors is evident in the triaxial case. The eigen-

tensor represents either triaxial tension or triaxial compression. For an eigenvector y_j of polar stretch S_{ij} of stiffness, in Mandel form, with the lowest eigenvalue, and its eigenvalue λ , both of the following are true:

$$S_{ij} y_j = \lambda \, y_j \tag{6.8}$$

$$S_{ij}\left(-y_{j}\right) = \lambda\left(-y_{j}\right) \tag{6.9}$$

Since the eigenvector multiplied by any constant satisfies the equations, the LAPACK library [3] may choose either case while solving the eigen decomposition. In order to correctly determine whether we have triaxial tension or triaxial compression, we need to do an additional test.

This test was suggested by Rebecca Brannon[1]. If we convert the Mandel eigenvector to its equivalent second-order symmetric eigentensor form Y_{ij} , we can test its "direction". It should be oriented during plastic loading such that,

$$\frac{\partial F}{\partial \sigma_{ij}} E^e_{ijkl} Y_{kl} > 0 \tag{6.10}$$

Here $\frac{\partial F}{\partial \sigma_{ij}}$ is the yield surface normal and E^e_{ijkl} is the elastic stiffness, for the particular integration point. If the condition in equation 6.10 is not satisfied, we multiply the eigentensor by -1. Then, it will have the correct orientation.

6.3.2.3 Polar Rotation and Elastic-Plastic Materials

The rotation part of the polar decomposition also carries interesting information. As we have mentioned in chapter 3, elastic-plastic materials are characterized by a yield function and a plastic flow potential function.

In associated material models, the yield surface and plastic flow surface coincide, and the plastic strain increment "direction" is the same as the "normal" to the yield surface[81]. Numerically, the yield surface normal is calculated as the partial derivative of the yield function with respect to stress, $\frac{\partial F}{\partial \sigma_{ij}}$. In associated materials there is no rotation component (**R** is the 6D identity matrix).

We conjecture that for *non-associated* materials, the polar rotation (in 6D) quantifies the degree of misalignment of the yield surface normal $(\frac{\partial F}{\partial \sigma_{ij}})$ and the plastic flow direction $(\frac{\partial G}{\partial \sigma_{ij}})$. In other words, we conjecture that applying the polar rotation to the yield surface normal produces the plastic flow direction to a good approximation. We confirmed this conjecture for some material models, as shown in the results section 6.6. However, it requires further empirical and theoretical evaluation.

6.4 Polar Decomposition Algorithm

One issue for polar decomposition on stiffness is that the matrix is not amenable to traditional numerical methods. During plastic yielding, the stiffness matrix can become positive semi-definite and therefore is not invertible; traditional methods use inversion. Moreover, the accompanying zero eigenvalue means that the polar decomposition is not unique. Although a general polar decomposition algorithm exists[31], we had already embarked on the creation of a new one that was much simpler and equally accurate for a single, near-zero or zero eigenvalue[58].

6.4.1 Simple Polar Decomposition for Positive-Definite Matrices

Van Gelder proposed the new algorithm[58], which I implemented, adding code to increase accuracy and debugging as I went along. The algorithm starts by finding the polar stretch **S** of stiffness matrix **E** and checking the number of near-zero or zero eigenvalues. We define D, and its relationship to the polar stretch S:

$$D = E^T E = S^T S = S^2 (6.11)$$

$$D = T J T^T \tag{6.12}$$

 \mathbf{T} 's columns are eigenvectors and \mathbf{J} is diagonal with sorted eigenvalues.

$$S = T \sqrt{J} T^T$$
 where \sqrt{J} is nonnegative (6.13)

$$S = \frac{1}{2}(S + S^T)$$
, improving accuracy (6.14)

If there are no zero or near-zero eigenvalues, the rotation \mathbf{R} can be calculated with an inversion:

$$R = E S^{-1} (6.15)$$

The correctness of the algorithm follows from **D**'s properties of being symmetric and positive semi-definite, and **T** being orthogonal so that $\mathbf{T}^T = \mathbf{T}^{-1}$.

6.4.2 Algorithm for a Zero or Near-Zero Eigenvalue

In the case of a zero or near-zero eigenvalue, the general idea is to use Gram-Schmidt completion to find the zero eigenvalue's column vector so that it is orthogonal to the others in \mathbf{T} , necessary for a rotation matrix. We can use the same method as shown in section 6.4.1 for calculating initial stretch \mathbf{S} , \mathbf{J} and initial \mathbf{T} . We start by defining a matrix variable \mathbf{C} in terms of \mathbf{T} . The goal is to find \mathbf{C} and use \mathbf{C} to calculate rotation \mathbf{R} . The steps of the algorithm are as follows:

$$C \equiv R T \tag{6.16}$$

$$B = ET = RST = R(T\sqrt{J}T^{T})T = C\sqrt{J}$$
(6.17)

Next, we calculate column vectors \mathbf{C}_j from column vectors \mathbf{B}_j , except the one corresponding to the zero eigenvalue:

$$C_j = B_j / \sqrt{J_{jj}} \quad \text{for } j = 2, \dots, n \tag{6.18}$$

Finally, we use Gram-Schmidt projection to get the final column of C

$$C_1 =$$
Gram-Schmidt completion of 6D orthonormal basis (6.19)

$$R = C T^T \tag{6.20}$$

$$S = sym\left(R^{-1}E\right) \tag{6.21}$$

The last step, enforcing symmetry, increases the accuracy of the stretch matrix.

6.4.3 Additional Details

When \mathbf{D} has a zero eigenvalue there can be either a negative or positive determinant for \mathbf{D} . We choose a positive determinant, as if the matrix had been positive definite. If the determinant is negative, we enforce this constraint by multiplying the first column of **T** by -1. (An eigenvector multiplied by any constant is also an eigenvector of a given matrix). This is done before the calculation B = ET in equation 6.17.

Additionally, to avoid dividing by zero in equation 6.18, we first make the zero eigenvalue of the diagonal matrix \mathbf{J} into a 1. In our implementation, we know that it corresponds to the first column of \mathbf{C} since the eigenvalues were previously sorted in ascending order.

Finally, we perform Gram-Schmidt on columns $2, \ldots, n$ and normalize them to make the orthogonalization more accurate. C_1 is then replaced with 1 for the first value and zero for the rest as a normalized "guess" vector before completing the Gram-Schmidt projection.

6.5 Analysis of Rotation Representation

In order to understand and analyze the rotation portion of the polar decomposition of the elastic-plastic stiffness, we need to look at how elastic-plastic stiffness is calculated.

In classical non-associative plasticity (without elastic-plastic coupling), the elastic-plastic stiffness tensor calculation is of the form

$$E_{ijkl}^{ep} = E_{ijkl}^{e} - (P_{ij}Q_{kl})/\eta$$
(6.22)

 \mathbf{E}^{e} is the symmetric, positive-definite elastic stiffness and $\mathbf{P}_{ij}\mathbf{Q}_{kl}$ is a dyad, and η is a scalar. This is the form found in the earthquake engineering simulator, OpenSees[62].

The dyad $\mathbf{P} \otimes \mathbf{Q}$ which has rank two (equal to that of \mathbf{P}_{ij}) even though $\mathbf{P} \otimes \mathbf{Q}$ is a fourth-order tensor. $\mathbf{P} \otimes \mathbf{Q}$ has a single non-zero eigenvalue and its eigentensor is equivalent to the first operand (\mathbf{P}) times a scalar. Subtracting a dyad from symmetric fourth-order tensor \mathbf{E}^e changes the stretch in at least one of its second-order eigentensors and potentially induces a rotation.

In the analysis, we show that the polar rotation rotates \mathbf{P} into \mathbf{Q} . However, we note that the rotation from \mathbf{P} to \mathbf{Q} is not unique.

6.5.1 Origin of Dyad Components

This section covers the origin of \mathbf{P} and \mathbf{Q} and η from equation 6.22. The section can be skipped if the details of solid mechanics modeling are not of interest to the reader.

In addition to the yield function $F(\sigma)$ and plastic potential function $G(\sigma)$, the simulator calculates the derivative of F and G and returns second-order tensors we will call A and B. These are respectively the yield surface "normal" and plastic potential surface "normal" described in section 6.3.2.3.

$$A = \frac{\partial F}{\partial \sigma_{ij}} \tag{6.23}$$

where F is the yield function.

$$B = \frac{\partial G}{\partial \sigma_{ij}} \tag{6.24}$$

where G is the plastic potential function.

Next, **A** and **B** are each contracted with the elastic stiffness \mathbf{E}^e .

$$P_{ij} = E^e_{ijkl} A_{kl} \tag{6.25}$$

$$Q_{kl} = B_{ij} E^e_{ijkl} \tag{6.26}$$

These are P and Q for our dyad $\mathbf{P} \otimes \mathbf{Q}$. The symbol η is a scalar of the form

$$\eta = H + A_{ij} E^e_{ijkl} B_{kl} \tag{6.27}$$

Here, H is the so-called ensemble hardening modulus (a scalar)[12].

For the remainder of the discussion, we will use equivalent 6D vectors with Mandel components for the equivalent symmetric second-order matrices (as shown in equation 5.3) and 6D matrices with Mandel components for fourth-order tensors with minor symmetry as shown in equation 6.6. The use of matrices and vectors allows the analysis to follow actual numerical implementation used in testing.

6.5.2 Justification for Rotation

This analysis came from Brannon. Let $F = P \otimes Q/\eta$. Substituting F into equation 6.22 gives

$$E^{ep} = E^e - F \tag{6.28}$$

Doing a polar decomposition on $E^e - E^{ep}$ is the same as doing a polar decomposition of F. F is not positive definite, so we have to use pseudo-inverses where an inverse is needed. Let F^T denote the transpose of F. Then

$$F^T F = ((Q \otimes P)(P \otimes Q))/\eta^2 = (pq/\eta)^2 (\hat{Q} \otimes \hat{Q})$$
(6.29)

$$FF^{T} = ((P \otimes Q)(Q \otimes P))/\eta^{2} = (pq/\eta)^{2}(\hat{P} \otimes \hat{P})$$
(6.30)

P normalized to unit length is \hat{P} , and **Q** normalized to unit length is \hat{Q} . \hat{P} is calculated $\frac{P}{p}$ where $p = \sqrt{(P_i P_i)}$, the magnitude. The scalar q likewise represents the magnitude of **Q**. Because of the nature of dyads, the fourth-order right and left polar stretch tensors are

$$U = (pq/\eta)(\hat{Q} \otimes \hat{Q}) \tag{6.31}$$

$$V = (pq/\eta)(\hat{P} \otimes \hat{P}) \tag{6.32}$$

We seek a rotation ${\cal R}$ such that

$$F = R S \tag{6.33}$$

$$F = V R \tag{6.34}$$

Writing these using $F=P\otimes Q/\eta$ and equation 6.31 gives

$$(P \otimes Q)/\eta = (pq/\eta)R(\hat{Q} \otimes \hat{Q})$$
(6.35)

$$(P \otimes Q)/\eta = (pq/\eta)(\hat{P} \otimes \hat{P})R \tag{6.36}$$

Dividing both sides by (pq/η) gives

$$\hat{P} \otimes \hat{Q} = R(\hat{Q} \otimes \hat{Q}) \tag{6.37}$$

$$\hat{P} \otimes \hat{Q} = (\hat{P} \otimes \hat{P})R \tag{6.38}$$

Finally, we note that

$$R(\hat{Q} \otimes \hat{Q}) = (R : \hat{Q}) \otimes \hat{Q} \tag{6.39}$$

and

$$(\hat{P} \otimes \hat{P})R = \hat{P} \otimes (\hat{P}:R).$$
(6.40)

Therefore, by omitting to take the same outer product on both sides of the equations:

$$\hat{P} = R : \hat{Q} \tag{6.41}$$

$$\hat{Q} = \hat{P} : R \tag{6.42}$$

This shows that the rotation tensor from pseudo polar decomposition of $\mathbf{E}^e - \mathbf{E}^{ep}$ defines the rotation of \hat{Q} into \hat{P} .

6.6 Results

We want to be able to test whether equation 6.41 and equation 6.42 hold for the material models in our earthquake engineering simulator. We start by normalizing \mathbf{P} and \mathbf{Q} from the simulator and call them \hat{P}_1 and \hat{Q}_1 .

$$\hat{P}_1 = \frac{P}{\|P\|}$$
(6.43)

$$\hat{Q}_1 = \frac{Q}{\|Q\|}$$
(6.44)

Next we rotate \hat{P}_1 and \hat{Q}_1 using the polar rotation matrix **R** of the elastic-plastic stiffness.

$$\hat{P}_2 = R : \hat{Q}_1 \tag{6.45}$$

$$\hat{Q}_2 = \hat{P}_1 : R$$
 (6.46)

We want to test how close the rotated matrices come to satisfying $\hat{P}_2 = \hat{P}_1$ and $\hat{Q}_2 = \hat{Q}_1$.

6.6.1 Testing Methods

I compared the second-order tensor \hat{P}_1 of equation 6.43 with \hat{P}_2 of equation 6.45 by two methods. The first method computes the Euclidean distance between the two tensors:

$$difference = \sqrt{\sum (\hat{P}_{ij1} - \hat{P}_{ij2})^2} \tag{6.47}$$

Since both tensors were normalized (magnitude of one) and the column vectors of R were normalized, the maximum possible difference was two.

The second method uses the definition of dot product

$$\hat{P}_1 \cdot \hat{P}_2 = |\hat{P}_1| |\hat{P}_2| \cos \theta \tag{6.48}$$

The difference between tensors is defined as the angle θ between \hat{P}_1 and \hat{P}_2 . If \hat{P}_1 and \hat{P}_2 are the same, θ is zero and the maximum difference is 2π radians. Although this definition was originally applied to vectors, we apply it here to second-order tensors. I applied the same tests to \hat{Q}_1 of equation 6.44 and \hat{Q}_2 of equation 6.46.

6.6.2 Tests of Material Models

We took measurements from similar simulations with three material models: an associated material (Drucker-Prager), a non-associated material (Drucker-Prager with a Von-Mises yield surface), and a non-associated material with elastic-plastic coupling(Dafalias-Manzari).

In the case of Drucker-Prager, A and B were equivalent and all of the rotations were the identity matrix. A and B represent the yield surface "normal" and plastic potential surface "normal" as described in section 6.3.2.3. If A is equivalent to B, then \hat{P}_1 is equivalent to \hat{Q}_1 . This was exactly what we expected for an associated material and clearly equations 6.45 and 6.46 were satisfied with an identity matrix for the rotation. The Euclidean test resulted in all zero values and the values for θ were all near zero within numerical precision.

For the first non-associated material (Drucker-Prager with a Von-Mises yield surface), the results were quite interesting. Figures 6.2 and 6.3 show results for step 124, the final step in the simulation.



Figure 6.2: Non-Associated Model, θ between rotated \hat{Q} and \hat{P}

The histograms show two distinct buckets, at zero and 1.26 radians. However, if we show only the cases where the rotation is *not the identity*, the zero bucket alone remains. (See figure 6.4).

The significance for this is that in the calculation of stiffness, below a certain threshold, only the elastic stiffness is used. Non-associativity still holds in \hat{P} and \hat{Q} , but they are not used in the calculation of stiffness. The stiffness is elastic (fully symmetric



Figure 6.3: Non-Associated Model, θ between rotated \hat{P} and \hat{Q}



Figure 6.4: Non-Associated Model, θ difference between rotated \hat{P} and \hat{Q} for non-identity rotations

and positive definite) and its polar rotation is the identity. Therefore, when the stiffness is elastic and the material is non-associated, the polar rotation does not reflect the rotation between \hat{P} and \hat{Q} .

Finally, we see a full range of values for Dafalias-Manzari, with two peaks (figure 6.5). We have shown the data set using Euclidean difference rather than θ because 0-100% can be more easily mapped to a 0-2.0 range. We expected the main bucket to have shifted right of zero at least 10% (mapping to 0.2 in the given range)

due to elastic-plastic coupling. Instead we see 2 peaks, near 0.4 and at 2.0, and a full spectrum of values. Thus, there are additional factors that remove this model from the class that can get a meaningful rotation from the polar decomposition of stiffness.



Figure 6.5: Dafalias-Manzari model, Euclidean difference between rotated \hat{Q} and \hat{P}

Chapter 7

Visualization of Second-Order, 3D, Non-Positive-Definite Symmetric Tensors

Chapter 4 details previous work with glyph, hyperstreamline and topology approaches for visualizing second-order symmetric tensor fields. Most fall short in addressing the needs of solid mechanics engineering because they do not find features of interest to the domain, or are limited to positive-definite or 2D tensors. In this chapter, we start with the features of interest and then present some new visualization approaches, experiments and results.

7.1 Stress and Strain Tensor Features

Tensor fields resulting from Geomechanics computations are mostly related to the state of stress (s_{ij}) and strain (ϵ_{ij}) . Both are symmetric, and non-positive definite. Stress is characterized by five basic modes, and a stress tensor may represent a pure mode or some combination of them. (Strain can likewise be characterized). The modes are:

- 1. spherical tension (three equal positive eigenvalues).
- 2. spherical compression (three equal negative eigenvalues).
- 3. triaxial compression (two equal eigenvalues with the distinct eigenvalue more compressive than the repeated eigenvalues).
- 4. triaxial tension (two equal eigenvalues with the distinct eigenvalue less compressive than the repeated eigenvalues).
- 5. pure shear (one zero eigenvalue, with the others equal and opposite in sign).

An isotropic stress (with three equal eigenvalues) corresponds to pressure which is equal from all directions. This case is similar to isotropy for DT-MRI [79] but can represent either compression (negative eigenvalues) or tension(positive eigenvalues). Triaxial tension or compression produces an axisymmetric stress (symmetric about one axis) and it is characterized by two equal eigenvalues. A state of pure shear stress is where one eigenvalue is zero and the other two are equal and opposite in sign.

7.1.1 Stresses in Geomaterial Solids

Stress tensors are of particular importance in solid mechanics, and Geomechanics as well, as they are useful as failure indicators. A large majority of Geomechanics theories deal with elastic-plastic behavior and failure of solids. Failure is based in stress space, putting a strong emphasis on understanding of stress tensor field. According to Jeremić, Geomechanics uses stress tensors to understand the behavior of soil and objects embedded in the soil as support for structural elements above. For example, concrete piles support buildings, bridges, or water tanks. The main features of interest are:

- Zones with positive stress (tension), particularly in piles. Tension results in cracking concrete.
- Zones with large shear stresses. In soil this can cause large shear deformations and shear failure.
- Zones of sign changes. A sudden switch from compressive to tensile behavior results in tensile failure.

Concrete and soils can withstand large compressive forces but fail under tension or in shear [39, 40, 36, 41]. These critical features are usually present at the interface between stiff concrete piles and soft surrounding soil, but they can occur anywhere in the solids[60].

7.2 Reynolds Glyphs

We used Reynolds glyphs to visualize the mode of stress that a solid is vulnerable to after it reaches the yield point. This was a test for the decomposition method represented in chapter 6. We hoped the visualization would show (a) regions that had become less stiff and (b) the mode of stress that would cause maximum deformation in those regions.

Reynolds glyphs visually depict characteristic modes of stress or strain [6]. The formula for a point on the surface of the second-order Reynolds glyph, using tensor notation from chapter 2 is:

$$c = n_i \,\sigma_{ij} \,n_j \tag{7.1}$$

Here, i, j range over 1, 2, 3 and 1, 2, 3 are Cartesian axes. n represents a 3D normalized vector of the direction cosine perpendicular to the plane of interest. In other words, each vector n represents a point on a unit sphere centered at (0, 0, 0).

Reynolds glyphs, coupled with color mapping, can clearly distinguish the five modes of stress. For instance, isotropic tension would be represented as a red sphere, and isotropic compression would be a blue sphere. For triaxial tension or triaxial compression, formula 7.1 produces an axisymmetric Reynolds glyph. The axis of symmetry is aligned with the eigenvector of stress corresponding to the distinct eigenvalue as shown in figure 7.1b. The disk shape in figure is similar to planar anisotropy for DT-MRI second-order tensors, also characterized by two equal eigenvalues [79].



Figure 7.1: Reynolds Glyph representations of modes of stress. Cool colors (blue and cyan) represent negative values, hot colors (red and yellow) represent positive. The X, Y, and Z axes are red, green, and blue respectively.

Pure shear produces a glyph such as the one in figure 7.1c. The distinct butterfly appearance of pure shear is caused by equal magnitude and opposite values across orthogonal directions on a single plane. This is the plane where shearing occurs; in this example it is the X - Y plane.

7.2.1 Graphical Issue

One graphical issue for Reynolds glyph arises when the scalar value c stretching the vector n is negative. The direction of the vector is reversed, and calculating the correct surface normal is more difficult. However, since the underlying tensor is symmetric, we can assume the glyph will be likewise symmetric. We can draw the point and calculate the surface normal without reversing the direction of n since both n and -n are on the surface of the glyph. We simply color them both with the magnitude of c.

7.2.2 Associated Scalar Color Fields

As noted in chapter 6, under sufficient stress a solid can yield, experiencing permanent deformation. When this happens, one or more eigenvalues reduce in magnitude. To find regions losing stiffness, we use the lowest eigenvalue from the decomposition of stiffness detailed in chapter 6. Coloring by minimum eigenvalue highlights regions where significant loss of stiffness and permanent deformation have occurred.

We also use the Lode angle θ , a stress invariant, to classify the mode of deviatoric stress[51, 56]. The original use for Lode angle was in the formulation of yield functions for isotropic solid material models, as well as others based on stress eigenvalues[12]. (More details on the yield function can be found in chapter 6.) The Lode angle is formulated:

$$\theta = \frac{1}{3} \sin^{-1} \left[\left(\frac{J_3}{2} \right) \left(\frac{3}{J_2} \right)^{\frac{3}{2}} \right]$$
(7.2)

 J_2 is the deviatoric stress invariant

$$J_2 = \frac{1}{2} \parallel S \parallel^2 \tag{7.3}$$

where **S** is the deviatoric part of the stress tensor σ_{ij} .

$$S_{ij} = \sigma_{ij} - \frac{1}{3}\sigma_{kk}\delta_{ij} \tag{7.4}$$

Here δ_{ij} is the Kronecker delta, the 3x3 identity matrix. J_3 is the determinant of S_{ij} . Figure 7.2 shows a yield surface (zero isosurface of the yield function) for a typical geomaterial, and a slice of the surface. The coordinate system is the orthogonal eigenvectors ("stress space") rather than Cartesian. The slice illustrates the continuous and reflective nature of the classification scheme despite ordering of eigenvalues.



Figure 7.2: Yield Surface (Stress-Space Isosurface) for an isotropic material and Lode angles for single slice. Image source: [12] TXE stands for triaxial extension, TXC is triaxial compression, SHR is shear, BXC is biaxial compression, and BXE is biaxial extension.



Figure 7.3: Lode Angle Color Scale and Glyphs

Figure 7.3 shows a rainbow color mapping of Lode angle, and the glyph shapes associated with the scalar values.

7.2.3 Experiment

We tested our technique on two simple experiments from Geomechanics. Both experiments consisted of 224 finite elements, each with 8 integration points on an irregular grid; a total of 1792 points for the volume. The experiments were run on OpenSees, a finite-element simulator for performance of structural and geotechnical systems subjected to earthquakes [62]. Data for the visualization was gathered during the runs, which took 10.5–12 minutes on an Intel 6600 2.4 Ghz dual core desktop with 2.0 gigabytes of RAM. The visualization runs at 1–4 frames per second, depending on the window size. Excerpts are shown in the figures. The software and experiment scripts are available from the authors and will soon be available through the VEES project website [57].

The experiments started with self-weight analysis of the soil, compressing along -Z, for 25 time steps. This is a common practice when studying soil behavior. The initial compression from the soil's own weight induces deformation and may also change the stiffness, depending on the model. The second part of the experiment was two point loads on the top of the volume. The loads included a small component along -Z (0.9659 kiloNewtons) and a large lateral component (1294 kiloNewtons). This part of the experiment ran for another 100 steps. Figure 7.4 shows the volume colored by displacement (Euclidean distance from initial position) on the last time step. The black arrows point to where the loads were applied along +X. In Figure 7.5a, 7.5b, 7.6a and 7.6b, we drew glyphs for each integration point in the volume, and the glyph size



Figure 7.4: Deformation (Euclidean distance), time step 124. Arrows indicate location and direction of applied point loads. Drucker-Prager material model.

was scaled by the size of the encapsulating finite element. These eigentensor glyphs were colored by the lowest eigenvalue and scaled across all time steps to give an overall idea of softening or hardening. In the case where the solid had not started permanent deformation (yielded), we drew spheres to indicate the elastic, isotropic material model. We used a black cube for the case of a negative eigenvalue in the stiffness tensor so the engineers could quickly identify singularity and the inability of the simulator to produce the mode of the instability.

The first soil material was Drucker-Prager. The material simply fails under tension, but it remains unchanged under compression (a "non-hardening" material). There were no changes in material stiffness during the self-weight steps. The material lost stiffness during the point load stress regime in the neighborhoods around and beneath the point loads, as shown in figure 7.5a. The mode of stress the solid became vulnerable to was similar to applied stress in the regions with loss of stiffness; triaxial compression in front of the point loads along the X axis, shear along the sides of the point loads and between them, and triaxial tension behind the applied loads. The user can quickly pick out these modes with Lode angle coloring (see figure 7.5b). Blue and cyan highlight the compression in front of the point loads, yellow trailing behind indicates tension, and green indicates shear. In this simple example, glyphs show a clear change in orientation and indicate principal stress directions (eigenvectors).



Top view (from +Z), Lode angle scalar coloring.

Figure 7.5: Drucker-Prager material model, time step 124.

The second simulated material was Dafalias and Manzari's plasticity sand model [15]. The model's stiffness is pressure-dependent and non-associated. In order to make the experiment repeatable we used the material constants given in the article, with the exception of the initial void ratio (e_0) . This material softens when it is denser (with smaller void ratios). Since we wanted to test our method's ability to detect softening, we reduced e_0 to 0.65. In this experiment, self-weight induced hardening. The greatest hardening occurred at the bottom of the volume, where the finite-element nodes were fixed and experiencing the greatest load from above. At first, stiffness increased with the depth of the volume, as expected with self-weight loading. With continued self-weight, loss of stiffness occurred in the volume we saw some integration points with negative eigenvalues. As the experiment continued, loss of stiffness occurred along the side boundaries of the volume, but there was frequent change between elastic and elastic-plastic states. It was difficult to correlate the stress to the behavior because of the changing yield surface and non-associativity. However, we did notice loss of stiffness on the top surface near the applied point loads late in the experiment (Figure 7.6a).



Lowest eigenvalue log scalar coloring.

Lode angle scalar coloring.

Figure 7.6: Dafalias-Manzari material model, time step 124.

7.3 Plane-In-A-Box Glyph

The motivation for our new glyph, plane-in-a-box, is to visualize high shear (both orientation and magnitude) as well as discriminate tension versus compression. The plane-in-a-box glyph is quite similar in appearance to tensor ellipsoids for the case when there is strong planar anisotropy. This glyph presents the same amount of relevant information as tensor ellipsoids using a simpler representation.



(a) (b) Single plane in enclosing box. Side view of a volume of plane-in-the-box glyphs.

Figure 7.7: Plane-in-a-box glyph.

The idea of plane-in-a-box is to create a plane with limited extent at each sample point. The size of the planar glyph is limited by a box whose edges are half the distance to each of the neighboring points. If the point is on a face of the volume, we simply extend it out a distance to half the distance of the neighboring interior point. Occlusion is reduced by scaling the planar glyphs while maintaining the general orientation. We opted for this simpler glyph since we are primarily interested in regions characterized by high shear. Pure shear exists on a single plane, and both triaxial tension and triaxial compression have a planar component. Thus, mapping the tensors to planar glyphs is quite natural. The plane spans the eigenvectors associated with the largest (major) eigenvalues, and the plane normal implies the eigenvector direction associated with the smallest (minor) eigenvalue. The plane itself can also be colored or filtered according to scalar parameters of interest. We explore the use of four scalars in the hope that they will help us find features of interest, namely: high shear, tension, and changes from compression to tension.

7.3.1 Data Structures and Algorithms

The plane-in-a-box glyph has two requirements. First, the sampled points must lay on a mesh, preferably a grid (although the grid need not be regular). In either case some connectivity among sample points is necessary to establish the locations of the edges of the box. For rectilinear data, we simply sort the points by the Z, Y, and X axes during preprocessing. Once the points are read in, we can deduce connectivity of neighboring points by checking the next and previous row, column, and slice.

We came to realize that finite element results do not necessarily lie on straight lines, as shown in 7.13. There are pie-shaped elements and variable sizes. For these data sets we take advantage any type of regularity that exist. In our case, slices on the Z plane were regular distances apart. We run Delaunay triangulation on the remainder to get connectivity. For both cases, connectivity is stored in an adjacency list.

7.3.1.1 Creating the Box and Finding Edge-Plane Intersections

The first step in creating glyphs is to create the box whose edges will limit the plane. By iterating through the linked list of rectilinear neighbors, we can determine the minimum and maximum X,Y, and Z distances to neighbors. We set box edges at half the distance to the neighbors and can even reduce the scale of the distance, if desired.



Figure 7.8: A box is formed around a point, based on the location of neighboring points.

For Delaunay neighbors we use a slightly simpler technique. We check the distance to each neighbor and select the one that is closest. We halve the distance and set that as the bounding distance along axes for which we have no rectilinear distances. This gives us good guarantees against polygon overlap although it may not be proportional to distance between points in all three directions.

Once we have the distances, we set the corners of the box using a lookup table which matches minimum or maximum X,Y, and Z to each box corner.

The next step is to create the plane, finding which edges of the box it intersects

and where on the edge the intersection occurs. We have a plane defined using pointnormal form, where the normal is the eigenvector corresponding to the minor eigenvalue. We convert it to general form

$$Ax + By + Cz + D = 0 \tag{7.5}$$

where A, B, and C are the X, Y, and Z components of the normal respectively. With the sample point at x_0, y_0, z_0 ,

$$D = (-1 * norm[X] * x_0) - (norm[Y] * y_0) - (norm[Z] * z_0)$$
(7.6)

Then, for each edge of the box, we use Bourke's algorithm [9] to find the intersection by extending the edge until it touches the plane.

$$P_{intersect} = t(P_2 - P_1) \tag{7.7}$$

where P_1 and P_2 are the points forming an edge of the box as shown in figure 7.9.

Substituting $t(P_2 - P_1)$ into our implicit plane equation yields

$$A(x_1 + t(x_2 - x_1)) + B(y_1 + t(y_2 - y_1)) + C(z_1 + t(z_2 - z_1)) + D = 0$$
(7.8)

and solving for t gives

$$t = \frac{Ax_1 + By_1 + Cz_1 + D}{A(x_1 - x_2) + B(y_1 - y_2) + C(z_1 - z_2)}$$
(7.9)



Figure 7.9: Intersection of plane and box edge. P_0 is the Gauss point.

The intersection occurs at $P_1 + t(P_2 - P_1)$. Once we have an intersection, if it lies on the edge between P_1 and P_2 , we update the box's edge index and store the intersection point in its marching cubes array.

In summary, we begin by creating a box which is limited by half the distance its neighbors. We calculate A, B, C, and D for our plane, based on the point location and its normal. Then we check each edge of the box to see if the plane intersects it, saving the intersection point $P_{intersect}$ and building an edge intersection case index. Finally, the edge intersection index is cross-referenced to a Marching Cubes index [52].

7.3.1.2 Marching Cubes for Simple Planes on an Irregular Grid

After extracting the intersections of the planes with the edges of the cell containing the tensor, the next step is the creation of the triangles that make up the plane. Our algorithm uses a variation on the well-known Marching Cubes [52].

Our algorithm differs in two ways:



Figure 7.10: Marching Cubes cases. (256 total with symmetry). Source: [52].

- 1. The index is built on edge intersections rather than a boolean for above or below an isovalue.
- 2. The box is composed of variable-sized quadrilaterals rather than a cube.

We deal with the first item by creating a mapping from each of the 256 marching cubes case indices to its corresponding edge index and save them in our reverse lookup table. More specifically, we iterate through each marching cubes triangle case array, building an active edge index. Then we make a hash table with the edge index as the key and the marching cubes index as the value, for fast retrieval. Figure 7.11 shows an example mapping. The hash table is used just before the call to marching cubes. Below is the pseudo code for the algorithm.

```
int plane_in_a_box(int i)
{
  calculate A, B, C, D
  make_box( i, box, plane_in_a_box_scale );
  for( j = 0; j < 12; j++ ) /* box edges */
  {
    calculate t</pre>
```



Figure 7.11: Mapping from plane-edge intersection to Marching Cubes index

```
calculate edge-plane intersection
```

```
if ( intersection is within edge )
 {
  /* copy edge intersection:
   2 out of 3 dimensions identical */
   mc_edges[j][X] = box[cube_edges[j][1]][X];
   mc_edges[j][Y] = box[cube_edges[j][1]][Y];
   mc_edges[j][Z] = box[cube_edges[j][1]][Z];
   mc_edges[j][edge_dim[j]] =
            touch_plane[edge_dim[j]];
    /* update edge case */
    index = index + CASE_INDEX[j];
   }
}/* for each box edge */
/* cross reference MC index */
index = get_value( MC_hash, index );
marching_cube( i, index, mc_edges );
```

}

Despite our box forming a hexahedron instead of a regular cube, we have found that marching cubes works quite well. Two facts help us. First, when we form the box around a sample point on the plane, we guarantee the box will enclose the plane. Second, because we build the case using a plane that spreads to the limits of the box, we never see the ambiguous marching cubes indices. Simply, since we build a continuous surface, we do not have holes. However, two other types of ambiguous cases



Figure 7.12: Sliding the box (brown to blue) to resolve case of edge lying in the plane.

can occur. One case is where an edge of the box lies in the plane. For such a plane, there are an infinite number of intersection points for the edge and the plane. Furthermore, three edges will claim intersection for each corner of the edge in the plane. In this case, a proper marching cubes index cannot be formed. The second ambiguity is where the plane intersects an edge at a box corner. As with the previous case, three edges will claim intersection for each corner of the edge in the plane. The simple solution is to shift the box a tiny amount along one axis and recalculate. We found this solution effective; we selected the first of multiple possible case indices, and shifted the box back before building the plane's triangles.

We predicted that we would see just a few different marching cubes cases as the point would sit in the middle of the box. This soon proved wrong as the sample point may lie almost anywhere within a skewed box.
7.3.2 Associated Scalar Color Fields

Stress features of interest for Geomechanics include tension, shear, sudden changes from compression to tension. We test four scalar measures for color mapping, opacity and filtering the plane glyphs. We provides several different scalar measures to aid exploration of a data set, and filtering mechanisms to home in on areas of interest in the volume. Three of the scalar measures come from Seismology and the fourth from tensor topology.

The scalar features are (i) signed isotropy (with both linear and log scaling), which is equivalent to spherical tension and compression from solid mechanics (ii) Seismic Double Couple (DC), which is equivalent to pure shear from solid mechanics (iii) Seismic Compensated Linear Vector Dipole which is equivalent to triaxial tension or triaxial compression from solid mechanics. (iv) Eigen difference [84].

7.3.3 Seismic Moment Tensors

Seismologists use a seismic moment tensor M_{ij} for a general representation of the seismic source [19]. Seismic moment tensors, like stress tensors, are symmetric and non-positive-definite. However, they differ in a couple of very important ways.

Seismic moment tensors or acoustic emission moment tensors are created from a measured event such as an earthquake or cracking solid. Sound waves are emitted at the event and can be measured. Thus, one major difference is that moment tensors represent a strictly *elastodynamic* source [43]. Second, in Geomechanics, a stress tensor relates to forces applied on the exterior surface of a volume. Moment tensors instead relate to forces that cause displacement across an *internal* surface, where the internal surface represents a buried fault [2].

Dreger et al. note that \mathbf{M}_{ij} is commonly decomposed into isotropic, double couple (DC) and compensated linear vector dipole (CLVD) components, where each of the components of the moment tensor decomposition is represented as a percentage of the total [19, 46, 43]. The same numerical features select for spherical tension/compression, shear, and triaxial tension/compression respectively. At the time this research was performed, however, we were not yet aware of the basic categories of mechanical stress, as described in section 7.1.

7.3.3.1 Isotropic and Deviatoric Components

Finding these scalar components starts with finding the eigenvectors and eigenvalues of $\mathbf{M}_{ij} = T J T^T$. A diagonalized moment tensor \mathbf{J} can be further decomposed into isotropic and deviatoric parts. A purely isotropic tensor is characterized by three equal eigenvalues. The isotropy in a moment tensor represents a change in volume. Pure isotropy in a moment tensor is comparable to an ideal explosion (positive eigenvalues) or implosion (negative eigenvalues) [20]. The equivalent for stress is spherical tension or compression. The isotropic portion is the identity matrix scaled by the mean of the three eigenvalues. The deviatoric component is the remainder of the original matrix after the isotropic component has been removed.

Below is the mathematical notation for the isotropic and deviatoric components of matrix J, where the trace (tr) is the sum of the diagonal elements and m_i^* is J_{ii} – tr(J)/3. Here, m_1^* has the smallest absolute magnitude and m_3^* the largest.

$$J = \begin{bmatrix} \frac{tr(J)}{3} & 0 & 0\\ 0 & \frac{tr(J)}{3} & 0\\ 0 & 0 & \frac{tr(J)}{3} \end{bmatrix} + \begin{bmatrix} m_1^* & 0 & 0\\ 0 & m_2^* & 0\\ 0 & 0 & m_3^* \end{bmatrix}$$
(7.10)

7.3.3.2 Two Vector Dipoles

Moment tensor elements represent dipoles. A dipole is composed of two equal and opposite vectors laying along an axis orthogonal to both of them. The physical meaning is the direction and angle of tectonic plate movement along opposite sides of a fault. According to Dreger, *double couple* (DC) consists of two linear vector dipoles of equal magnitude but opposite sign, resolving shear motion on faults. The shear is oriented 45 degrees to the principal eigenvectors of M_{ij} [19]. In mechanical terms, if the force in the double couple exceeds a material's threshold, a shearing event will occur [20], or displacement along the fault plane (parallel to the largest stress). In a pure DC event, the eigenvalues are proportional to 1, 0, -1 [43]. In this section we use DC and pure shear interchangeably.

Compensated linear vector dipole (CLVD) refers to when "a change in volume is compensated by particle motion in the plane parallel to the largest stress" [20]. This may be a mechanism for deep earthquakes [46]. CLVD is modeled by eigenvalues proportional to -2, 1, 1, reflecting particle motion. Figure 4.9 shows the failure mechanisms associated with pure isotropy, DC, and CLVD.

The contribution of DC and CLVD to the deviatoric component of a moment

tensor can be calculated as follows: For components of the diagonalized moment tensor without isotropy, m_1^*, m_2^*, m_3^* such that

$$|m_3^*| \ge |m_2^*| \ge |m_1^*| \tag{7.11}$$

$$F = -\frac{|m_1^*|}{|m_3^*|} \tag{7.12}$$

F is the ratio of the smallest to largest absolutes of the eigenvalues and we expect a value of 0.0 for pure DC and 0.5 for pure CLVD. Note that **F** does not distinguish triaxial compression $(m_i^* \propto (1, 1, -2))$ and triaxial tension (eigenvalues $m_i^* \propto (-1, -1, 2)$). However, one could examine the sign of m_1^* , and create a scalar that gives similar information to the Lode angle.

Assuming the deviatoric is a result of only DC and CLVD,

$$m_{deviatoric} = m_{deviatoric} = m_{deviatoric} = m_{3}^{*}(1-2F) \begin{bmatrix} 0 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + m_{3}^{*}F \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$
(7.13)

For scalar features there are two quantities:

$$DC = m_3^*(1 - 2F) \tag{7.14}$$

$$CLVD = m_3^*F \tag{7.15}$$

Following Anderson and Finck [4, 20], percentage of deviatoric that is CLVD can be calculated:

$$\frac{2m_3^*F}{|2m_3^*F| + |m_3^*(1 - 2F)|}\tag{7.16}$$

The CLVD is doubled so there can be a range of 0.0 - 1.0 instead of 0.0 - 0.5. We use the estimate $\parallel 2\mathbf{F} \parallel$ for culling and coloring glyphs for simplicity.

Zheng, et al. categorized double degenerate points in a second-order symmetric tensor field by first sorting eigenvalues by absolute magnitude: $|\lambda_1| \ge |\lambda_2| \ge |\lambda_3|$. *Planar* degenerate points had $|\lambda_1| = |\lambda_2| \ge |\lambda_3|$ and *linear* degenerate points had $|\lambda_1| \ge |\lambda_2| = |\lambda_3|$. [84]. They proposed a scalar K as:

$$K = 2\lambda_2 - (\lambda_1 + \lambda_3) \tag{7.17}$$

where K is a positive value for planar degenerate tensors (identical major and medium eigenvalues), and a negative value for linear degenerate tensors (identical medium and minor eigenvalues). We were curious to see how the scalar would operate on our tensor field.

7.3.3.3 Scalar Calculation and Meaning

We built an application with a menu for selecting a feature for coloring the planes and a feature for setting plane opacity.

Since the two features, DC and CLVD, can be expressed as percentiles, they are automatically scaled from 0 to 1. For isotropy and eigen difference, we set the zero valued features (the midpoint) at 0.5. We scaled cool colors (blue) below, from 0.5 to 0 for negative values and hot colors (red) for positive values scaled up from 0.5 to 1. Opacity can provide some filtering effect as the lowest values are fully transparent. Medium to high values appear more solid and their geometry is highlighted, similar to volume rendering, and we mapped scalars to opacity with the same scale.

The application also has sliders for selecting a range of values for features. For example, a user can select strictly positive isotropy combined with high CLVD. Such combinations allow users to search for domain-specific indicators. The aforementioned, for example, can signify a crack when the data set is composed of moment tensors from acoustic emissions [20]. With thresholding, the shape of regions are also clearly delimited. Essentially, the user can create isosurface and iso-volume-like selections. However, the surface is not smooth, being composed of individually oriented planes. Finally, the application can show the *inverse* of a selected feature range, providing greater flexibility.

7.3.3.4 User Interaction

Rather than thresholding over the entire volume, a user may wish to explore from points of interest on outwards. We provide a pointer that the user can move around the volume to select various seed points. Then, on each iteration, neighboring planes get painted. This gives an animation effect of oriented planes growing out of the seed point. Thresholding constraints may also be applied, as desired. For this type of interaction, we built two data structures that save state between animation frames. One is a draw list where each entry refers to a sample point in the volume. This is initialized to all zeros to indicate no planes should be drawn; only non-zero entries have their planes drawn during an iteration. The second is a queue that holds the sample point numbers to be added to the draw list on the next iteration. In addition, the point adjacency is stored in an adjacency list, implemented as an array of linked lists. The algorithm proceeds as a simple breadth first traversal. At first glance, the extra complexity may seem unnecessary; after all, for regular data we can simply use the stride of the length, width, and slice of the rectilinear sorted data. However, in many cases, Geomechanics data is *not* regular. Gauss points across finite elements are not lined up along X and Y, as shown in figure 7.13. We would still like to explore a region from a selected seed point, and breadth first traversal of the mesh works well for this.

After initialization with the user's selected seed points, we take each point from the queue, add it to the draw list, and check its linked list of neighbors. Here again, we depend on having neighbor connectivity available. We do a check three things before we consider adding a new point to the next iteration's queue. The sample point must meet all of the user's constraints, and neither the current draw list nor the current queue may already contain it.

The data structures and process are very similar to Gibson's Chainmail algorithm [23]. The Chainmail algorithm enables fast deformation of volumetric objects, composed of objects such as nodes and points from Finite Element analysis. The analogy is that points and nodes move as if joined by a chain link mesh. If a node is moved beyond a constraint, neighboring nodes will also move. Similarly, on each iteration of our algorithm, new candidates are queued breadth-first and previously selected candidates are tested against the constraints.

7.3.4 Data Meaning

The particular data sets used in this paper are related to two applied Geomechanics problems. The first data set represents a finite sized model with two point loads on top, the Boussinesq problem (i.e. [50]). The problem is simple enough that the results are known in advance and represents an excellent verification procedure. In addition, symmetry planes in the model can be used for verification of numerical and visualization procedures.

The second data set is from a dynamic, seismic bridge simulation. It represents a stress field from one time step of an elastic-plastic, dynamic simulation of a soil– foundation–structure (SFS) bridge system [8, 7]. This data set involves large ratios of stresses between stiff concrete in columns of the main structure, and the soft soil beneath. In addition, the main characteristics of the stress fields are not known in advance as we use simulations to gain a better understanding of the behavior of the SFS system and the interactions of its components during seismic events.

7.3.5 Data Representation

The volume of the bridge–soil system is built from finite elements. Each element has a hull of vertex *nodes* that may be shared with neighboring elements. The shape of an element need not be rectilinear. Within each element are *gauss points*. That is, the Gaussian method is used to locate points that produce the most accurate



Mesh of Finite Elements



Gauss point

Figure 7.13: Finite Element Data Set

integration.

As the simulation progresses, nodes move, inducing stress at the gauss points. Hence, the stress tensor field consists of the induced stresses at these gauss points.

7.3.6 Results

We tested our application using two data sets, each of which was a single time step in a Geomechanics simulation. Both data sets consisted of a field of stress tensors for geomechanical soils and solids, as described in section 7.3.5.

The first was the Boussinesq point load, where force was applied at two points on the top of the volume. The second was a bridge supported by two piles in soil. In the simulation, force was applied to one side of the bridge, followed by seismic shaking.

7.3.6.1 Boussinesq Point Load

Figure 7.14a shows isotropy in the double point load data set. Linear scaling of the color map highlights the compressive and tensile forces at the points they were applied.

The eigenvalues at these points were extremely high, so the linear scale caused the rest of the volume to appear to have zero isotropy evenly throughout. However, when we change to a log scale and scale the opacity as well, the variation from negative to positive is strongly emphasized (Figure 7.14b). Here, advantage of the isotropy scalar is clear. It shows not only the type of stress, but also its degree. There is high tension (positive isotropy) below one point load, high compression below the other, and a mixture on the surface.





Linear rainbow scale color, arrows show applied loads

Log scale color and opacity.

Figure 7.14: Boussinesq dual point load, isotropy color map



Figure 7.15: Double point load, DC color map (CLVD is the dual and has the same appearance but with blue instead of red)

Figures 7.15a, b, and c show the coloring for the double couple feature (1.0- || F ||). The range of colors tells us that the anisotropy types range from pure shear (DC) to midway between pure shear and triaxial tension or compression(CLVD). We omitted CLVD since it is calculated as the dual of DC and would appear as blue–green color mapping instead of green–red. It is clear regions with the pure shear feature are distinct from regions with high isotropic tension or compression.

In Figures 7.15b and c, we see the results of DC thresholding. Both figures show greater than 50% similarity to the DC feature, but the first figure has a color representing lower similarity overall. We found it interesting that using a lower threshold selected the very noisy data around the points where stress was applied. The region most closely matching a DC feature was where we expected the shear to occur – on the plane between where

the two opposing forces were applied. Combinations of constraints on several types of features may lead to better understanding of stress within a volume, in addition to a scalar representing magnitude of anisotropy. For example, isotropic stress is largest at the point where the loads are applied (Figure 7.14). The DC feature is strongest on the plane between the two opposite loads, a very different region of the volume (Figure 7.15c). Positive isotropy in combination with anisotropic behavior might lead to fracture.

7.3.6.2 Bridge Pile Data Set

Figures 7.17a and b show the entire volume for bridge supports embedded in soil. The piles penetrate halfway down onto the soil. In the simulation, the applied force, shown as the yellow arrow in figure 7.17a, pushed the bridge support to the right. The expected behavior is is that the left side of the pile will be under tension and the right side under compression, as shown in figure 7.16. The eigen difference coloring



Figure 7.16: Yellow arrow shows applied pushover force. Red arrows show resulting tension, and blue arrows show compression.

highlights the changes in stress with red and blue coloring above the surface and within the piles. The sharp red-blue contrast along the upper neck of the piles and in the bridge emphasizes that type of stress is flipping from linear to planar. In figure 7.17b, within the neck of the piles, there is a red line indicating high DC. Therefore, there is pure shear occurring at the location of the flip.



Figure 7.17: Bridge Data Set.

There is a circular appearance in the planes' orientation at the center of the volume. This is attributable to boundary effects in the simulation and represents a very important finding as it tells us that the model needs to be enlarged in order to more realistically simulate the half-space. Figure 7.18 shows thresholding by isotropy. This is an example of using the inverse of a threshold range, eliminating everything in the range from 0.25-0.75. The figure is colored by log scale isotropy and shows ranges of 0.0-0.25 representing compression and 0.75-1.0, representing tension. The bridge pile on the right has a color change from red to blue just above where the pile enters the soil, indicating that the stress has switched from tension to compression. This is one of the critical features in Geomechanics that can result in tensile failure. The isotropy figure also shows a



Figure 7.18: Bridge data set, log scaled isotropy, 0.0-0.25 and 0.75-1.0

shadowing effect. Shadowing comes from an analogy between the applied force and light, where a supporting member may absorb or block the force. Its shadow is an area under less stress. The shadowing is indeed interesting as it directly and visually conveys information about an important physical behavior, namely the back bridge support will be shadowed by the front bridge support, and savings can be made in reinforcement steel for shadowed bending.

Figure 7.18 also presents a visual proof that the model can and needs to be extended in the horizontal direction in order to simulate the half space more realistically. Ideally, the simulation would be sufficiently large that the boundaries would be unaffected by the applied force. However, this is always a tradeoff with computation cost and even with this smaller model we can get meaningful results.

7.3.7 Conclusions

One of the goals of plane-in-a-box was to find planes of shear. This was accomplished in the case of pure shear or DC, where there is one zero eigenvalue and shearing occurs in the plane of the two eigenvectors with non-zero eigenvalues. Here, using the zero eigenvalue's eigenvector as the plane normal makes perfect sense. In the case of CLVD, there is not a single shearing plane. Maximum shear occurs at 45° from the plane of eigenvectors with equal eigenvalues. In this case it might make more sense to visualize the planar part (the plane of eigenvectors with equal eigenvalues) or use a different type of glyph than a plane. No planar glyph makes sense for pure isotropy.

Isotropy turned out to be the most useful feature among those we tried. Along with thresholding, it highlighted information about the materials' physical behavior under stress. The scalar K was the least useful as it could really only apply to positive definite data. Both triaxial compression and triaxial tension are by the definition planar degenerate, yet have K values of opposite sign; both should have a positive K value.

7.4 Continuous Visualization

Continuous visualization such as hyperstreamlines have been used successfully for fluid dynamics data, DT-MRI data, and 2D stress tensor fields. In this section, we explore approaches to visualizing stress, strain or stiffness eigenmode tensor fields using a continuous visualization.

7.4.1 Interpolating to a Regular Mesh

One issue for continuous visualization of these tensor fields is that the finite element method is often used for simulation. Finite elements, as shown in figure 7.13, are irregularly shaped and can simulate discrete material types. Stiffness may not cross element boundaries, and we do not want to assume a continuity that may not exist. Therefore, interpolation needs to respect boundaries of the finite elements.

The basic algorithm is:

```
For each point location within the volume {
   Find finite element enclosing point location
   Get tensor at each Gauss integration point within element,
   and its Cartesian location.
   for each tensor component {
      Run Shepard's interpolation algorithm on component.
   }
}
```

This algorithm runs in $O(G^*E)$ where G is the number of regular grid points and E is the number of finite elements. We used a simple caching method to improve performance; we tested whether the current point location is in the same element as previous, before

doing a brute force search.

7.4.2 Creating an Eigenvector Field

There are two issues for 3D hyperstreamlines. First, one must choose one of three hyperstreamlines, major, medium or minor. Secondly, Zheng et al. note it is generally impossible to sort the eigenvalues in a consistent and continuous fashion and hence the hyperstreamlines, while continuous, may exhibit sudden changes in directions [84].

We propose that the significant eigenvector for a point in the volume of solid mechanics data depends on the type of stress at the point, and should be chosen relative to maximum shear. We can use the Lode angle θ to ascertain the anisotropic stress type. This is calculated directly from the tensor, and the angle θ ranges from -30° (triaxial compression) to $+30^{\circ}$ (triaxial tension), with 0° indicating pure shear. This is shown in figure 7.2. If the eigenvalues are sorted in ascending order (but not by absolute value), it is very easy to select the eigenvector of interest.



Figure 7.19: Reynolds glyphs, and the maximum shear directions for each stress mode, and the eigenvector selected based on Lode angle.

The algorithm has four simple cases:

• $(\theta \leq -10)$

Triaxial compression, sorted eigenvalues (-2,+1,+1)

Use first eigenvector, associated with smallest eigenvalue

• $(\theta > -10 \&\& \theta \le +10)$

Pure shear, sorted eigenvalues (-1, 0, +1)

Use second eigenvector, associated with middle eigenvalue

• $(\theta > +10)$

Triaxial tension, sorted eigenvalues (-1,-1,2)

Use third eigenvector, associated with largest eigenvalue

• Isotropic stress (three equal eigenvalues)

All possible sets of three orthogonal vectors are eigenvectors of the tensor. None is significant. Possible approaches include halting the hyperstreamline, or continue it on its previous trajectory with a shape or color change indicating isotropy.

The reason these eigenvectors are of interest is that shear occurs in a consistent direction relative to the eigenvector associated with the selected eigenvalue. Pure shear occurs in a plane orthogonal to the selected eigenvector. Shear associated with triaxial tension or triaxial compression occurs 45° off from the selected eigenvector. Figure 7.19 shows



Figure 7.20: Drucker-Prager Stiffness Eigenmode field, colored by Lode angle.

Reynolds glyphs with maximum shear drawn in black. Eigenvectors selected by the Lode angle criterion are shown. Figure 7.20 shows an example of such an eigenvector field using eigenmode from Drucker-Prager stiffness.

7.4.3 Future Work

The name of the proposed visualization is "Necklaces". The "string" of the necklace is a hyperstreamline, and the "beads" on the necklace are glyphs that show stress type and maximum shear orientation, when viewed from any direction (see figure 7.21). Spherical tension and compression will be represented as spheres (no shear), pure shear as planes with lines indicating the directions of maximum shear. Triaxial tension and compression will have cones oriented along the eigenvector associated with the largest absolute value. The surface of the cone will be along the direction of maximum

shear (45° off from eigenvector with the largest absolute eigenvalue). Using parameters, it will be possible to change continuously between the three shapes. Filtering can be used to find the stress types of interest.



Figure 7.21: Glyph and tensor line "necklace".

There are two advantages in this approach:

- The "beads" along the necklace reduce the difficulty of following tensor lines' orientation. For example, perspective viewing will change the size of the beads as they recede from the user's viewpoint.
- 2. In regions where stresses have similar orientation, a pattern will emerge along the orientation of maximum shear. The pattern is due to the effects of reification (Gestalt psychology), where an object is perceived as having more spatial information than is present in the original stimulus.

This technique will be both visually appealing and useful. It will show one of the principal stresses, direction of maximum shear, and stress type. Scalar color mapping can show one additional attribute (such as magnitude of maximum shear or isotropy) and be used for filtering.

Chapter 8

Documentation of VEES Software

8.1 Introduction

This section of the thesis provides documentation of the software, VEES[59](Visualizer for the Earthquake Engineering System), developed to support the research. It includes a user guide and architecture documentation.

We planned to address visualization of finite element solid mechanics data by providing a general application to allow exploration of a simulation domain. Additionally, we planned to provide a means for the user to focus on a specific element within a domain and new techniques to show the critical details at the location. The hope is that we will come to understand what is important to observe at both levels and so help future users to more easily find the "good and the bad stuff".

The main theme, for usability, is Shneiderman's well known three level approach from information visualization: overview, zoom and filter, and details-on-demand



Figure 8.1: VEES visualization environment.

[71].

VEES plugs into the object-oriented OpenSees[62] finite element simulator. OpenSees contains natural hierarchies of Finite Element Types such as volume elements (Bricks), beams, and trusses and Materials representing soil, concrete, steel, etc. The simulator immediately provides all geometry as well as associated scalar and tensor data. The theme for the VEES architecture is the Strategy design pattern[21] (using an interchangeable family of algorithms, for visualization).

8.2 User Guide

8.2.1 Linux Setup and Getting Started

It is necessary to have GLUT and GLUI 2.2-2.2 libraries installed in addition to the modified version of OpenSees and its required libraries.

OpenSees can be run as a command line or by using tcl scripts. Modify your own tcl scripts by adding the command, vees The vees command does not get loaded into OpenSees until after the model is declared, e.g.

model BasicBuilder -ndm 3 -ndf 3

Calling vees should then give you the graphical user interface, but to see your mesh, call vees after creating your nodes and elements. Note: when vees closes it will also close OpenSees.exe (a bug!)

Execute OpenSees to start. When your script reaches the vees command it will open a window and 2 floating menus.

The last section of this chapter contains an example script.

8.2.2 Using VEES

In any of the vees display windows, you can interact by placing the mouse in the display window and using the following keyboard commands:

- [x] rotate about x axis
- [y] rotate about y axis
- [z] rotate about z axis

- [+] zoom in
- [-] zoom out
- [r] reset to original orientation

Clicking an eight node brick will show the selected element in the upper right hand *Element* window.

Clicking an integration point on the element window will show details in the *Integration Point* window.

8.2.3 Main Window

In the rendering control window you can choose from a drop down menu of drawing methods.

Rendering Con 💷 🗙				
	Draw Function: Mesh	a		
	Max Color 1.0	Mesh		
	Min Color 0.0	Displaced Mesh		
	Invert Color Range	Solid		
	Hide Element Type –	Displaced Solid		
	EightNodeBrick ElasticBeam3d	Gauss Points		
	Select Element: 0	Stiffness		

Figure 8.2: VEES render mode controls.

Select one of the draw functions from the drop down menu. You can select from several coloring schemes at the bottom of the main window. Each is scaled into into a 0 to 1 range, where 0 is blue, 0.5 is green, 1 is red. Element Type assigns each element type a unique random color.

Displacement is the Euclidean length of the displacement vector, i.e. $\sqrt{\sum (v[i] * v[i])}$ from each degree of freedom *i* up to the number of dimensions of the node (2 or 3). **Gauss Points** are compatible with stress color functions only. **Stiffness** is compatible with stiffness color functions only.

8.2.4 Filtering

There are two types of filters to explore the data:

- By value: you can limit the upper and lower value using the Max Color and Min Color spinners, and also invert the range (show everything outside the selected range)
- By element type: check the box for the element type you would like to hide.

8.2.5 Color Map Range Adjustment

At the bottom left, there is a widget set for color maps. You can select the color map from the drop down list. The range for the color map is set to the (absolute) maximum for the current time step. If the values for the time step are all very small (absolute value between 0 and 1.0) the the color map range maximum is set to 1.0.

You can adjust the color map range by clicking on the text area, using the backspace key to remove old digits and then typing in new ones. Sometimes it sticks a little, just click another part of the interface and click back to make it work.

Color Map Range +/- D12 Function: Displacement C Linear scale C Log scale	Node Number Element Number Element Type Displacement Mean Stress Deviatoric Stress Min Stiffness Stiffness
	Stiffness Eigenmode

Figure 8.3: Select coloring scheme, adjust range and select linear or log scale.

Log scale is useful if the color map range covers several orders of magnitude, such as for mean stress.

8.2.6 Element Window

There are two ways to select an element to view in the element window.

- 1. Click on the element in main window. (Note that you can only click surface elements. If you need an interior element you will have to filter first).
- 2. Type the element number in the **Select Element** text box in the Render Controls widget.

You can then click one of the element's integration points to view in the Integration Point Window. The selected point will be highlighted in red.

8.2.7 Integration Point Window

This windows shows Reynolds glyphs for tensor data. There are keyboard commands to view stress and various aspects of stiffness.

To view the stress tensor, type \mathbf{G} .



Figure 8.4: Element Viewer. Selected integration point highlighted in red.

To view the stiffness tensor, type 7.

There are several view types of the eigentensors of stiffness. The default is the eigen decomposition of the polar stretch of stiffness.

Type 8 to view the eigentensors on the non-decomposed stiffness.

Type \mathbf{S} to change to eigentensors of the *symmetric part* of stiffness.

Type 9 to switch back to eigentensors of the *polar stretch*.

The numbers **0-5** display glyphs of the 6 eigentensors for the selected decomposition type. Type **0** to see the eigentensor with the lowest eigenvalue. The eigentensors are ordered from lowest eigenvalue to highest.

8.2.8 Capturing Images and Data for Post-Processing

I have added an OpenSees recorder command that records all node data (degrees of freedom, etc.) and stress, strain, and stiffness for many elements and materials. The command is

recorder domain <-file \$filename>

Specifying the file name is optional. The default file names will be domain1, domain2, etc. Be careful, the files can be quite large for the 3D soil materials.

The files can then be reloaded using the widget shown in figure 8.2.8.

Load Step		_ • ×
File domain Save Image Save SVTK Save Stress Save Eigentensor	Load	> >>

Figure 8.5: Widget for replaying times steps.

You can load a specific time step by entering the step number in the text area under the load button and clicking **Load**. To move to the next time step, click the >button. Use the < button to load the previous step.

To run through many time steps as a movie, enter the first time step in the text area below the Load button and the last time step in the text area labeled **End Step**. Then click the \gg button to run forward, or \ll to run backwards.

I find it useful to load the last time step, set the color map ranges, and then run through the time steps as a movie.

Save the images click the Save Image checkbox before loading time steps. It

is also possible to save stiffness, stress, polar rotation, and the eigentensor associated with the lowest eigenvalue by clicking the checkboxes. The tensors are interpolated (component by component) to a regular grid.

8.3 Architecture

VEES acts as a plug-in to OpenSees. OpenSees is an object oriented C++ Finite Element simulator with Tcl wrappers. The data types organized in natural hierarchy of elements such as beams or soil volume elements, as well as material models for concrete, soil, steel, etc. A subset of the hierarchy is shown in figure 8.3. The container for these is an object called the Domain. VEES has access to the Domain, its



Figure 8.6: OpenSees Domain class, its component Elements, and their component materials.

components, and their data, as shown in the UML diagram (figure 8.3.1. It is organized using several well-known design patterns, and some of the pattern applications are novel. OpenSees contains multiple data sets we would like to visualize (stress, strain, stiffness, deformation), and we would like to be able to visualize each data set in multiple ways.

8.3.1 Model-View-Controller

The model-view-controller is a pattern for user interface design[47]. The idea is to have separate objects for the application (the Model), its screen presentation (the View), and the Controller which defines reaction to user input. Its purpose is to facilitate multiple views of the same data set. We followed this pattern closely. The Model is the OpenSees Domain, which holds instances of all nodes and Finite Elements, as well as their data.



Figure 8.7: UML diagram of VEES.

The main window is an instance of GlutWin, which uses the GLUT window-

ing library and GLUI widget library. It has four subwindows as shown in figure 8.1. Each subwindow had a VisWin instance which encapsulates a Viewer and a Camera, and shared access to the Domain. The VisWin acts as a graphic Controller, handling lighting, centering, projection, picking, rotation, zoom, and requests to filter the data shown. Its Viewer is responsible for extracting data from the Domain and drawing it. The simple hierarchy of Viewers is shown in figure 8.3.1. You can see that the Viewers facilitate overview of all Finite Elements (DomainViewer) to full details at a single Gauss integration point (GlyphViewer). This is evident in the user interface, as shown in figure 8.1.

All the Viewers communicate with the GlutWin main window, but the DomainViewer is the major work horse. It encapsulates arrays of DrawElement objects and color maps, saves data to files, loads time steps and refreshes its view.

8.3.2 Strategy Pattern

The main theme for VEES is the Strategy design pattern[21], using an interchangable family of algorithms for visualization. We accomplished this through a single level hierarchy of class DrawElement as shown in figure 8.3.2. The DomainViewer con-



Figure 8.8: DrawElement class hierarchy.

tains an array of each type of DrawElement, and iterates through the selected array on

a call to draw. This displays each finite element, as shown in the code snippet below:

```
ElementIter &theElements = theDomain->getElements();
while (( theElement = theElements->next() ) != NULL) {
   drawMethods[theElement->getTag()]->drawElement(
       theElement, color[theElement->getTag()],
       ranges[currRange],drawStyle );
}
```

The DrawElement type, color map, and filtering range are all parameterized. The DrawElement subclasses are self-explanatory except for HideElement, which exemplifies the Command pattern[21].

8.3.3 Command Pattern

One filtering mechanism provided in VEES is filtering by Finite Element type, as shown with checkboxes in figure 8.2. We want to be able to iterate through the



Figure 8.9: Substituting a HideElement instance for a DrawWireFrame instance, and saving a reference to the old DrawWireFrame instance so we can revert back to it later.

elements and draw them, but we need a way to skip over the filtered elements. When drawing is based on a scalar value, it is simple to check the scalar against the color map range during iteration. But in the case filtering by Finite Element type, this will not work. We use the Command pattern[21], encapsulating the request to hide the element as an object. "Undo" means again drawing the object as it was drawn previously.

When an element type is selected for hiding, for each instance of that element we substitute a HideElement instance. Since we want to be able to "undo" the hiding, we need to save the old drawing object. The HideElement interface has a setLastDrawnAs(DrawElement *) method, and a revert() method that returns the old DrawElement.

8.3.4 Memento

We extend VEES and OpenSees to provide visualization during and or after a simulation run. Our lightweight framework leverages existing superclasses within OpenSees while providing the necessities save time steps and reload in a series or individually. We apply the Momento design pattern[21], serializing objects' state so that it can be saved in a file and restored, without breaking objects' encapsulation.

We add two classes to OpenSees, DomainRecorder and File_Channel. Domain-Recorder is a subclass of the OpenSees Recorder. Recorders perform some action on each commit step in a simulation, usually saving some type of data to a file.

Our DomainRecorder records the current state of the entire simulation domain (stress, strain, stiffness, deformation). In other words, it serializes all the components (Elements, Materials) and their state to a file. The DomainRecorder takes advantage an interface(MovableObject) that all components in the Domain must implement. MovableObjects must implement two methods

- sendSelf(int commitTag, Channel &theChannel) which serializes the object's state and sends it through a Channel which may represent a file, socket, datebase, etc.
- recvSelf(int commitTag, Channel &theChannel, FEM_ObjectBroker &theBroker) which reads state from a Channel and reinstantiates the object via a Broker.

The interface was originally designed to assist with parallelization, by serializing objects to send to other compute nodes. We use it instead to send state to file on each commit step. The state of the entire simulation Domain is saved to file using the existing sendSelf methods.

VEES loads Domain state in a similar fashion, using recvSelf. The graphical user interface facilitates incrementing and decrementing time steps, or running an entire simulation as a movie, as shown in figure 8.2.8. Each time we load a time step, the Domain runs recvSelf on all its components. Then we propogate the update to each of the Viewers. They reread the data from the Domain, and refresh the drawing.

8.4 OpenSees Example

#(jeremic,zhyang)@ucdavis.edu
tcl example file using Template3Dep material
Inelastic static analysis -- Triaxial test
#two load stages:
stage 1: isotropic compression

stage 2: triaxial shearing

```
#-----
# create the modelbuilder
#-----
model BasicBuilder -ndm 3 -ndf 3
set g 9.81
# ------
# build the model
# -----
node 1 1.0 1.0 0.0
node 2 0.0 1.0 0.0
node 3 0.0 0.0 0.0
node 4 1.0 0.0 0.0
node 5 1.0 1.0 1.0
node 6 0.0 1.0 1.0
node 7 0.0 0.0 1.0
node 8 1.0 0.0 1.0
```

triaxial test boundary

fix 1 0 1 1
```
fix 2 1 1 1
fix 3 1 0 1
fix 4 0 0 1
```

```
# Linear elastic --id-Youngs--poisson--rho
nDMaterial ElasticIsotropic3D 2 70000 0.2 1.8
```

nDMaterial Template3Dep 1 2 -YS \$ys -PS \$ps -EPS \$EPS -ELS1 \$ES1 -ELT1 \$ET1 # tag 8 nodes matID bforce1 bforce2 bforce3 rho element Brick8N 1 5 6 7 8 1 2 3 4 1 0.0 0.0 -9.81 1.8

#stage 1

#isotropic load

set p 5.0

set np -5.0

pattern Plain 2 "Linear"

load 1 \$np 0 0 -pattern 2

load 3 0 \$p 0 -pattern 2

load 4 \$np \$p 0 -pattern 2

load 5 \$np \$np \$np -pattern 2

load 6 \$p \$np \$np -pattern 2

load 7 \$p \$p \$np -pattern 2

load 8 \$np \$p \$np -pattern 2

#Set up recorder

recorder domain

set lf1 0.01
set NN1 500
system UmfPack
constraints Penalty 1e12 1e12
test NormDispIncr 1.0e-8 30 1
integrator LoadControl \$lf1 1 \$lf1 \$lf1
algorithm Newton
numberer RCM
analysis Static
analyze \$NN1

NN1: number of iterations

#stage 2

#set previous load constant loadConst time 0 # Before shifting to disp. control, # apply reference load on the top pattern Plain 3 "Linear" load 5 0.0 0.0 \$np load 6 0.0 0.0 \$np load 7 0.0 0.0 \$np load 8 0.0 0.0 \$np load 1 \$p 0 0

#Set up recorder for axial loading stage recorder domain set NN2 1000 set ndz -0.0001 system UmfPack constraints Penalty 1e12 1e12 test NormDispIncr 1.0e-08 30 1 integrator DisplacementControl 5 3 \$ndz 1 \$ndz \$ndz algorithm Newton numberer RCM

analysis Static

analyze \$NN2

#visualize

vees

Chapter 9

Conclusion

In this dissertation, we have presented some novel approaches to visualizing stress, strain and stiffness tensors from solid mechanics. We have had some success in decomposing fourth-order stiffness tensors to facilitate their visualization, but further research is needed. Clearly, solutions to visualizing a wider range of material models' stiffness will depend on the models' formulation and meaning.

During the course of this research, a clearer picture has emerged of engineers' needs with regards to visualizing stress tensors. Since materials frequently fail under tension and in shear, shear planes, stress type and magnitude of stress invariants must all be part of the solution. We have solved different parts of the puzzle, and proposed future work that we expect will be a more complete and satisfactory solution.

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