Technical Appendix for "Decomposition and Visualization of Fourth-Order Elastic-Plastic Tensors"

These appendix sections provide additional technical details that could not be included in the proceedings paper, due to space limitations. In the interest of self-containment, we first review some tensor basics.

Tensor Notation and Operations

Tensors are linear operators that can be represented as multi-dimensional arrays of coefficients. For 3-D solids, a fourth-order tensor is a $3 \times 3 \times 3 \times 3$ array, a second-order tensor is a 3×3 array, etc. The order of a tensor is the same as the number of subscripts needed to write a typical element. Thus, if $\mathbf{E}$ is a fourth-order tensor, a typical element is denoted by $E_{ijk\ell}$. Scalars, vectors, and matrices represent tensors of orders zero, one, and two, respectively.

Operations using tensors are usually denoted using the *Einstein convention* that repeated indices in different tensors are implicitly summed; e.g., matrix multiplication is denoted as $C_{ij} = A_{ik} B_{kj}$, rather than the explicit equation,

$$C_{ij} = \sum_k A_{ik} B_{kj}. \tag{7}$$

This operation is called a *single contraction* in tensor terminology, and is often denoted by "·" as an infix symbol.

In elasticity (and many other physical processes) the *double contraction* operator is important. It is denoted by ":" as an infix symbol, and involves summing over two indices, e.g.,

$$C_{ij} = \mathbf{A} : \mathbf{B} = A_{ijk\ell} B_{k\ell} = \sum_k \sum_\ell A_{ijk\ell} B_{k\ell} \tag{8}$$

Double contraction can also be applied to two fourth-order tensors, yielding a new fourth-order tensor.

Where many operations on first and second order tensors use single summation, their generalizations to second and fourth order tensors use double summation. The above example of double contraction is thus the generalization of multiplying a matrix by a vector. Two important cases are the scalar *inner product*, $A_{ij} B_{ij}$, and the *dyad* or *outer product*, $A_{ij} B_{k\ell}$ that results in a fourth-order tensor.

Appendix A: Unrolling Plasticity Tensors to Matrices and Vectors

Operations on fourth-order 3-D tensors with minor symmetries are more conveniently computed and analyzed by a transformation to 6×6 matrices. Recall that the minor symmetries are $E_{ijk\ell} = E_{jik\ell} = E_{ij\ell k} = E_{ji\ell k}$. Symmetric second-order tensors are transformed into 6-vectors. As explained below, under this transformation, the usual linear-algebra vector and matrix operations correspond to the tensor operations involving double contraction (eq. 8); single contraction and dyad formation ("zero" contraction) also correspond to 6-D vector operations. This transformation is informally called *unrolling*.

Numerical methods for eigen-decomposition and polar decomposition only exist for matrices (rather than fourth-order tensors). Therefore it is computationally advantageous to represent second-order tensors as vectors and *linear transformations* on second-order tensors as matrices. (The natural representation of a linear transformation from second-order tensors to second-order tensors is a fourth-order tensor.)

The straightforward representation of a 3×3 tensor would be as a 9-vector with one component for each tensor element. As applied first by Jean Mandel, ("Ondes plastiques dans un milieu indéfini à trois dimensions," *Journal de Mécanique*, Vol. 1 (1962), pp. 3–30), and later rigorously justified by others, (see main paper for citations), due to the symmetry of the 3×3 tensor space of interest, an orthonormal change of basis can force the last three components of the 9-vector to be zero. This orthonormal change of basis in 9-D simply consists of 45° 2-D degree rotations on the three pairs of vector components that correspond to symmetric pairs of *off-diagonal* tensor elements.

Similarly, the straightforward representation of a *linear transformation* on 3×3 tensors would be a 9×9 matrix, but if the set of transformations is restricted to those that produce symmetric results, after applying the orthonormal change of basis, a 6×6 matrix suffices.

In summary, as long as the *physical quantities* of interest have the structure of symmetric 3×3 tensors, the corresponding vectors can be 6-D instead of 9-D, and linear transformations of such tensors can be represented with 6×6 matrices. Because the tensors used in the models we visualize always enjoy the minor symmetries, the transformation into 6-D suffices, and is described here.

The first part of the unrolling involves a mapping from single indices in the range $1, \ldots, 6$ into pairs of indices in the range $1, 2, 3$.

k	1	2	3	4	5	6
$\mu(k)$	$(1,1)$	$(2,2)$	$(3,3)$	$(1,2)$	$(2,3)$	$(1,3)$

(9)

Other orders of the last three pairs are acceptable, but one order must be used consistently. Note that μ^{-1} is well defined and maps pairs of indices into single indices. Minor symmetries dictate values for tensor elements whose index pairs do not appear in the table.

Let $\mathbf{I}_3$ and $\mathbf{0}_3$ denote the 3×3 identity matrix and zero matrix. With the above notation we define the 6×6 matrix $\mathbf{E}$ that represents the unrolling of the fourth-order tensor $E_{ijk\ell}$:

$$\mathbf{E} = \begin{bmatrix} \mathbf{I}_3 & \mathbf{0}_3 \\ \mathbf{0}_3 & \sqrt{2}\mathbf{I}_3 \end{bmatrix} \begin{bmatrix} E_{\mu(1),\mu(1)} & \cdots & E_{\mu(1),\mu(6)} \\ \vdots & & \vdots \\ E_{\mu(6),\mu(1)} & \cdots & E_{\mu(6),\mu(6)} \end{bmatrix} \begin{bmatrix} \mathbf{I}_3 & \mathbf{0}_3 \\ \mathbf{0}_3 & \sqrt{2}\mathbf{I}_3 \end{bmatrix} \tag{10}$$

Similarly, the 6-D column vector $\mathbf{s}$ that represents the unrolling of the second-order tensor S_{ij} is given by:

$$\mathbf{s} \;=\; \begin{bmatrix} \mathbf{I}_3 & \mathbf{0}_3 \\ \mathbf{0}_3 & \sqrt{2}\mathbf{I}_3 \end{bmatrix} \begin{bmatrix} S_{\mu(1)} \\ \vdots \\ S_{\mu(6)} \end{bmatrix} \qquad (11)$$

To recover tensors from matrices and vectors, simply use the inverse of the scaling matrix and the inverse of μ.

Appendix B: Polar Decomposition of Plasticity Matrices

Once we have a tensor in matrix form we can perform polar decomposition. The method described here is designed to be robust in the presence of a very small or zero eigenvalue. Experience has shown that another published method performs poorly in these situations. The method we use follows a recent paper (A. Van Gelder, "Relaxed Jordan Canonical Form for Computer Animation and Visualization," submitted for publication July 2008, available from the author), and is described here for self-containment. For our application, we assume that the matrix is square, the determinant is nonnegative, and there is at most one eigenvalue that is zero. In particular, we are not aware of any interpretation of the polar decomposition in this application when $\det \mathbf{E} < 0$, and do not perform polar decomposition in this case.

The polar decomposition on the $n \times n$ square matrix $\mathbf{E}$ is defined as

$$\mathbf{E} \;=\; \mathbf{QS} \qquad (12)$$

where $\mathbf{Q}$ is an orthogonal matrix and $\mathbf{S}$ is a symmetric positive semidefinite matrix. (Conventionally, the term "orthogonal" in this context includes the requirement that rows and columns be unit-length, besides being pairwise orthogonal.) If the determinant of $\mathbf{E}$ is nonnegative, then the determinant of $\mathbf{Q}$ is $+1$. The main paper cites previous methods in the literature, which are either more complicated or more restricted than the method we adopt, described below.

It is well known that the decomposition is unique for $\det \mathbf{E} > 0$. If $\mathbf{E}$ has one eigenvalue of 0, the decomposition is still unique with the specification that $\det \mathbf{Q} = +1$. (Proofs of this and other claims in the appendix are available from the authors in manuscript.) In all cases the $\mathbf{S}$ part of the decomposition is unique.

The steps are summarized in the following equations, where $\mathbf{Q}$ and $\mathbf{S}$ are unknown until they appear on the left side of an equation, and "$\equiv$ introduces a definition of an unknown. A single subscript on a matrix denotes a *column* of that matrix.

$$\begin{aligned}
\mathbf{M} &= \mathbf{E}^T\mathbf{E} \;=\; \mathbf{S}^T\mathbf{S} \;=\; \mathbf{S}^2 \\
\mathbf{M} &= \mathbf{T}\mathbf{J}\mathbf{T}^T && \text{where } J \text{ is diagonal, ascending order} \\
\mathbf{S} &= \mathbf{T}\sqrt{\mathbf{J}}\mathbf{T}^T && \text{where } \sqrt{\mathbf{J}} \text{ is nonnegative} \\
\mathbf{C} &\equiv \mathbf{QT} \\
\mathbf{B} &= \mathbf{ET} \;=\; \mathbf{QST} \;=\; \mathbf{C}\sqrt{\mathbf{J}} \\
\mathbf{C}_j &= \mathbf{B}_j / \sqrt{\mathbf{J}}_{jj} && \text{for } j = 2, \ldots, n \\
\mathbf{C}_1 &= \text{Gram-Schmidt completion of 6-D orthonormal basis} \\
\mathbf{Q} &= \mathbf{C}\mathbf{T}^T \\
\mathbf{S} &= \text{sym}\left(\mathbf{Q}^{-1}\mathbf{E}\right)
\end{aligned}$$

Higham recommends the same computation as the last line, except using $\mathbf{Q}^T$ in place of $\mathbf{Q}^{-1}$, and in theory they are equal. We obtain slightly more accuracy with $\mathbf{Q}^{-1}$. In the Gram-Schmidt completion on the next to last line, replace the column $\mathbf{C}_1$ with $-\mathbf{C}_1$ if $\det \mathbf{C}$ and $\det \mathbf{T}$ have opposite signs. The Jacobi method is very robust and accurate for the computation of eigenvalues and eigenvectors on the second line.

The correctness of the procedure is shown in the cited paper and follows from well known linear algebra properties of real symmetric matrices; in particular, $\mathbf{M}$ is positive semidefinite and $\mathbf{T}$ can be chosen to be orthogonal, so that $\mathbf{T}^T = \mathbf{T}^{-1}$.

As applied in this paper, $n = 6$ and the 6×6 matrix being decomposed is usually the plastic stiffness matrix, which results from unrolling the plastic stiffness tensor (see Appendix A). If there is an eigenvalue of zero for $\mathbf{S}$, its eigenvector is found in column one of $\mathbf{T}$; *in this case*, that column is also an eigenvector for the zero eigenvalue of the stiffness matrix and is of special interest. In addition, the matrices $\mathbf{T}$ and $\sqrt{\mathbf{J}}$, which are by-products of the decomposition procedure, are useful for various simulations.

Appendix C: Isotropic Stiffness Matrix

Many materials exhibit *isotropic* elasticity properties. For such materials the stiffness tensor can be expressed in terms of two parameters, K, the *bulk modulus*, and G, the *shear modulus*. The stiffness matrix (unrolled stiffness tensor, see Appendix A) for isotropic materials is given by

$$\mathbf{E} \;=\; \begin{bmatrix} K+\frac{4}{3}G & K-\frac{2}{3}G & K-\frac{2}{3}G & 0 & 0 & 0 \\ K-\frac{2}{3}G & K+\frac{4}{3}G & K-\frac{2}{3}G & 0 & 0 & 0 \\ K-\frac{2}{3}G & K-\frac{2}{3}G & K+\frac{4}{3}G & 0 & 0 & 0 \\ 0 & 0 & 0 & 2G & 0 & 0 \\ 0 & 0 & 0 & 0 & 2G & 0 \\ 0 & 0 & 0 & 0 & 0 & 2G \end{bmatrix} \qquad (13)$$

The eigen-decomposition for isotropic stiffness plays an important role in the visualization. One eigenvalue is $3K$ and the other five are $2G$. The eigenvector for $3K$ is $[1, 1, 1, 0, 0, 0]^T$. All 6-vectors orthogonal to this vector are eigenvectors for $2G$; they span a 5-D subspace.