POLAR DECOMPOSITION AND LOGARITHMIC STRAIN IN THREE DIMENSIONS

by
Stephen V. Harren
http://www.harren.us

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1. Introductory Comments

The material herein is for use in a three-dimensional finite element program for finite elasticity in three dimensions. Such a program, *i.e.,* `FiniteElasticity3D.java`, is located on this web site. When the author first started to write that program, he tried to do the required three-dimensional eigenproblems by using characteristic polynomials and rank-deficient systems to calculate the eigenvalues and eigenvectors. Such an approach turned out to be highly cumbersome and unreliable. Consequently, in the above-mentioned finite element program (again, on this web site), the author resorted to using Babylonian iteration to perform the polar decomposition, and to using a Taylor series expansion to calculate the logarithmic strain. While this approach is reliable, its numerical execution is rather slow. The procedures outlined below have also been found to be reliable, but numerically execute more quickly, and thus are probably superior to the Babylonian iteration/Taylor series procedures just described.

2. The Three-Dimensional Eigenproblem

Consider a three-dimensional, symmetric matrix A, *viz.,*

$$A = \begin{bmatrix} A_{00} & A_{01} & A_{02} \\ A_{01} & A_{11} & A_{12} \\ A_{02} & A_{12} & A_{22} \end{bmatrix} , \qquad A^E = \begin{bmatrix} \lambda_0 & 0 & 0 \\ 0 & \lambda_1 & 0 \\ 0 & 0 & \lambda_2 \end{bmatrix} , \qquad A = \psi^T A^E \psi \ , \qquad A^E = \psi A \psi^T \ , \quad (2.1)$$

where

$$\mathbf{e}_i^E = \psi_{ij} \mathbf{e}_j \ . \quad (2.2)$$

In eqns. (2.1) and (2.2), λ_i are the eigenvalues of matrix A, $\mathbf{e}_i^E$ are the corresponding eigenvectors, $\mathbf{e}_i$ are the Cartesian base vectors of three-dimensional space, and ψ is the rotation matrix.

The rotation matrix ψ can be constructed by performing three successive rotations about, in order, the x–, y– and z–axes. Thus

$$\psi^2 = \begin{bmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{bmatrix} , \quad \psi^1 = \begin{bmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{bmatrix} , \quad \psi^0 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\gamma & \sin\gamma \\ 0 & -\sin\gamma & \cos\gamma \end{bmatrix} \quad (2.3)$$

so that $\psi = \psi^2 \psi^1 \psi^0$, *i.e.,*

$$\psi = \begin{bmatrix} \cos\alpha\cos\beta & -\cos\alpha\sin\beta\sin\gamma + \sin\alpha\cos\gamma & \cos\alpha\sin\beta\cos\gamma + \sin\alpha\sin\gamma \\ -\sin\alpha\cos\beta & \sin\alpha\sin\beta\sin\gamma + \cos\alpha\cos\gamma & -\sin\alpha\sin\beta\cos\gamma + \cos\alpha\sin\gamma \\ -\sin\beta & -\cos\beta\sin\gamma & \cos\beta\cos\gamma \end{bmatrix} . \quad (2.4)$$

Also,

$$\frac{\partial\psi}{\partial\alpha} = \begin{bmatrix} -\sin\alpha\cos\beta & \sin\alpha\sin\beta\sin\gamma + \cos\alpha\cos\gamma & -\sin\alpha\sin\beta\cos\gamma + \cos\alpha\sin\gamma \\ -\cos\alpha\cos\beta & \cos\alpha\sin\beta\sin\gamma - \sin\alpha\cos\gamma & -\cos\alpha\sin\beta\cos\gamma - \sin\alpha\sin\gamma \\ 0 & 0 & 0 \end{bmatrix} ,$$

$$\frac{\partial\psi}{\partial\beta} = \begin{bmatrix} -\cos\alpha\sin\beta & -\cos\alpha\cos\beta\sin\gamma & \cos\alpha\cos\beta\cos\gamma \\ \sin\alpha\sin\beta & \sin\alpha\cos\beta\sin\gamma & -\sin\alpha\cos\beta\cos\gamma \\ -\cos\beta & \sin\beta\sin\gamma & -\sin\beta\cos\gamma \end{bmatrix} , \quad (2.5)$$

$$\frac{\partial\psi}{\partial\gamma} = \begin{bmatrix} 0 & -\cos\alpha\sin\beta\cos\gamma - \sin\alpha\sin\gamma & -\cos\alpha\sin\beta\sin\gamma + \sin\alpha\cos\gamma \\ 0 & \sin\alpha\sin\beta\cos\gamma - \cos\alpha\sin\gamma & \sin\alpha\sin\beta\sin\gamma + \cos\alpha\cos\gamma \\ 0 & -\cos\beta\cos\gamma & -\cos\beta\sin\gamma \end{bmatrix} .$$

To solve for the matrix ψ, use the last of eqns. (2.1), *i.e.*, $A^E_{ij} = \psi_{ik}\psi_{jl}A_{kl}$. Specifically, use the three components $(ij) \in (01{,}02{,}12)$ so that

$$0 = \psi_{ik}\psi_{jl}A_{kl} \ , \tag{2.6}$$

which is a nonlinear 3×3 system in the three variables α, β and γ. An effective means of solving eqn. (2.6) is to use Newton-Raphson iteration. Thus, we have the residual

$$r_{(ij)} = \psi_{ik}\psi_{jl}A_{kl} = 0 \ , \tag{2.7}$$

and, using the notation $(x_0, x_1, x_2) = (\alpha, \beta, \gamma)$, the iterative procedure

$$J_{(ij)m}\Delta x_m = -r_{(ij)} \ , \qquad {}^{\mathrm{imp}}x_m = x_m + \Delta x_m \ , \tag{2.8}$$

where ${}^{\mathrm{imp}}x_m$ is an improved guess for x_m. The Jacobian in eqn. (2.8) is

$$J_{(ij)m} = \frac{\partial r_{(ij)}}{\partial x_m} = \frac{\partial \psi_{ik}}{\partial x_m}\psi_{jl}A_{kl} + \psi_{ik}\frac{\partial \psi_{jl}}{\partial x_m}A_{kl} \ . \tag{2.9}$$

Reliable results are obtained by initially guessing that $x_m = 0$, and by iterating until $\sum_{i=0}^{3}|\Delta x_i| \le 10^{-7}$. So, knowing x_m, ψ is known, and once ψ is known, the eigenvalues are found from the components $(ij) \in (00{,}11{,}22)$ of $A^E_{ij} = \psi_{ik}\psi_{jl}A_{kl}$. Thus,

$$\lambda_i = \psi_{ik}\psi_{(i)l}A_{kl} \ . \tag{2.10}$$

In a numerical method for three-dimensional nonlinear elasticity, the gradients of λ_i and ψ_{ij} with respect to the components A_{pq} are required. Consequently, differentiation of eqn. (2.6) yields

$$0 = \frac{\partial \psi_{ik}}{\partial A_{pq}}\psi_{jl}A_{kl} + \psi_{ik}\frac{\partial \psi_{jl}}{\partial A_{pq}}A_{kl} + \frac{1}{2}\left(\psi_{ip}\psi_{jq} + \psi_{iq}\psi_{jp}\right). \tag{2.11}$$

Now, via the Chain Rule, $\partial\psi_{ij}/\partial A_{pq} = \left(\partial\psi_{ij}/\partial x_m\right)\left(\partial x_m/\partial A_{pq}\right)$, which when put into eqn. (2.11) gives

$$J_{(ij)m}\frac{\partial x_m}{\partial A_{pq}} = -\frac{1}{2}\left(\psi_{ip}\psi_{jq} + \psi_{iq}\psi_{jp}\right) \ , \tag{2.12}$$

where $J_{(ij)m}$ is as per eqn. (2.9) above. Finally, eqn. (2.12) may be solved for $\partial x_m/\partial A_{pq}$ so that the gradients $\partial\psi_{ij}/\partial A_{pq}$ are found. Knowing $\partial\psi_{ij}/\partial A_{pq}$, then differentiation of eqn. (2.10) gives the gradients of λ_i, *viz.*,

$$\frac{\partial \lambda_i}{\partial A_{pq}} = \frac{\partial \psi_{ik}}{\partial A_{pq}}\psi_{(i)l}A_{kl} + \psi_{ik}\frac{\partial \psi_{(i)l}}{\partial A_{pq}}A_{kl} + \psi_{ip}\psi_{(i)q} \ . \tag{2.13}$$

An advantage of the above method, as compared to the Babylonian iteration/Taylor series method described in Sec. 1, is that, once ψ is known, then the expressions for the gradients of λ_i and ψ_{ij} are in closed form.

As a numerical example, for

$$A = \begin{bmatrix} 3 & 2 & 1 \\ 2 & 8 & 5 \\ 1 & 5 & 4 \end{bmatrix} \ , \tag{2.14}$$

the above procedures yield

$$\psi = \begin{bmatrix} -0.146\,827 & 0.579\,220 & -0.801\,839 \\ -0.240\,972 & -0.807\,148 & -0.538\,929 \\ -0.959\,361 & 0.114\,092 & 0.258\,087 \end{bmatrix} ,$$

$$A^E = \begin{bmatrix} 0.571\,259 & 0 & 0 \\ 0 & 11.935\,6 & 0 \\ 0 & 0 & 2.493\,13 \end{bmatrix} . \tag{2.15}$$

One may verify that eqn. (2.15) satisfies $A = \psi^T A^E \psi$.

3. The Polar Decomposition Theorem

The Polar Decomposition Theorem states that

$$F = VR \ , \tag{3.1}$$

where F is the deformation gradient, V is the (symmetric) left stretch tensor (with positive eigenvalues), and R is the rotation tensor. Consider

$$B = FF^T = VRR^TV = VIV = VV \quad \Rightarrow \quad V = \sqrt{B} \ . \tag{3.2}$$

This square root is calculated via

$$B^E = \begin{bmatrix} \lambda_0 & 0 & 0 \\ 0 & \lambda_1 & 0 \\ 0 & 0 & \lambda_2 \end{bmatrix} , \quad B^E = \psi B \psi^T \ , \quad V^E = \begin{bmatrix} \sqrt{\lambda_0} & 0 & 0 \\ 0 & \sqrt{\lambda_1} & 0 \\ 0 & 0 & \sqrt{\lambda_2} \end{bmatrix} , \quad V = \psi^T V^E \psi \ . \tag{3.3}$$

Now, the gradients $\partial V_{ij}/\partial F_{pq}$ are required for use in a finite element code. Consequently, differentiation of $B = VV$ yields

$$\frac{\partial B_{ij}}{\partial V_{pq}} = \frac{1}{2}\left(\delta_{ip}V_{jq} + \delta_{iq}V_{jp} + V_{ip}\delta_{jq} + V_{iq}\delta_{jp}\right) \ , \tag{3.4}$$

where δ_{ij} is the Kronecker delta (*i.e.,* the 3×3 identity matrix). But, the quantities $\partial V_{pq}/\partial B_{kl}$ are needed, which quantities follow the inverse relation

$$\frac{\partial B_{ij}}{\partial V_{pq}} \frac{\partial V_{pq}}{\partial B_{kl}} = I_{ijkl} = \frac{1}{2}\left(\delta_{ik}\delta_{jl} + \delta_{jk}\delta_{il}\right) \ , \tag{3.5}$$

in which I_{ijkl} is the fully symmetric fourth-order identity tensor. Equation (3.5) can be written in matrix form as

$$\left[\frac{\partial B}{\partial V}\right]\left[\frac{\partial V}{\partial B}\right] = I_{6\times 6} \ , \tag{3.6}$$

where

$$\left[\frac{\partial B}{\partial V}\right] = \begin{bmatrix} \frac{\partial B_{00}}{\partial V_{00}} & 2\frac{\partial B_{00}}{\partial V_{01}} & 2\frac{\partial B_{00}}{\partial V_{02}} & \frac{\partial B_{00}}{\partial V_{11}} & 2\frac{\partial B_{00}}{\partial V_{12}} & \frac{\partial B_{00}}{\partial V_{22}} \\ 2\frac{\partial B_{01}}{\partial V_{00}} & 4\frac{\partial B_{01}}{\partial V_{01}} & 4\frac{\partial B_{01}}{\partial V_{02}} & 2\frac{\partial B_{01}}{\partial V_{11}} & 4\frac{\partial B_{01}}{\partial V_{12}} & 2\frac{\partial B_{01}}{\partial V_{22}} \\ 2\frac{\partial B_{02}}{\partial V_{00}} & 4\frac{\partial B_{02}}{\partial V_{01}} & 4\frac{\partial B_{02}}{\partial V_{02}} & 2\frac{\partial B_{02}}{\partial V_{11}} & 4\frac{\partial B_{02}}{\partial V_{12}} & 2\frac{\partial B_{02}}{\partial V_{22}} \\ \frac{\partial B_{11}}{\partial V_{00}} & 2\frac{\partial B_{11}}{\partial V_{01}} & 2\frac{\partial B_{11}}{\partial V_{02}} & \frac{\partial B_{11}}{\partial V_{11}} & 2\frac{\partial B_{11}}{\partial V_{12}} & \frac{\partial B_{11}}{\partial V_{22}} \\ 2\frac{\partial B_{12}}{\partial V_{00}} & 4\frac{\partial B_{12}}{\partial V_{01}} & 4\frac{\partial B_{12}}{\partial V_{02}} & 2\frac{\partial B_{12}}{\partial V_{11}} & 4\frac{\partial B_{12}}{\partial V_{12}} & 2\frac{\partial B_{12}}{\partial V_{22}} \\ \frac{\partial B_{22}}{\partial V_{00}} & 2\frac{\partial B_{22}}{\partial V_{01}} & 2\frac{\partial B_{22}}{\partial V_{02}} & \frac{\partial B_{22}}{\partial V_{11}} & 2\frac{\partial B_{22}}{\partial V_{12}} & \frac{\partial B_{22}}{\partial V_{22}} \end{bmatrix} , \tag{3.7}$$

and

$$\left[\frac{\partial V}{\partial B}\right] = \begin{bmatrix} \frac{\partial V_{00}}{\partial B_{00}} & \frac{\partial V_{00}}{\partial B_{01}} & \frac{\partial V_{00}}{\partial B_{02}} & \frac{\partial V_{00}}{\partial B_{11}} & \frac{\partial V_{00}}{\partial B_{12}} & \frac{\partial V_{00}}{\partial B_{22}} \\ \frac{\partial V_{01}}{\partial B_{00}} & \frac{\partial V_{01}}{\partial B_{01}} & \frac{\partial V_{01}}{\partial B_{02}} & \frac{\partial V_{01}}{\partial B_{11}} & \frac{\partial V_{01}}{\partial B_{12}} & \frac{\partial V_{01}}{\partial B_{22}} \\ \frac{\partial V_{02}}{\partial B_{00}} & \frac{\partial V_{02}}{\partial B_{01}} & \frac{\partial V_{02}}{\partial B_{02}} & \frac{\partial V_{02}}{\partial B_{11}} & \frac{\partial V_{02}}{\partial B_{12}} & \frac{\partial V_{02}}{\partial B_{22}} \\ \frac{\partial V_{11}}{\partial B_{00}} & \frac{\partial V_{11}}{\partial B_{01}} & \frac{\partial V_{11}}{\partial B_{02}} & \frac{\partial V_{11}}{\partial B_{11}} & \frac{\partial V_{11}}{\partial B_{12}} & \frac{\partial V_{11}}{\partial B_{22}} \\ \frac{\partial V_{12}}{\partial B_{00}} & \frac{\partial V_{12}}{\partial B_{01}} & \frac{\partial V_{12}}{\partial B_{02}} & \frac{\partial V_{12}}{\partial B_{11}} & \frac{\partial V_{12}}{\partial B_{12}} & \frac{\partial V_{12}}{\partial B_{22}} \\ \frac{\partial V_{22}}{\partial B_{00}} & \frac{\partial V_{22}}{\partial B_{01}} & \frac{\partial V_{22}}{\partial B_{02}} & \frac{\partial V_{22}}{\partial B_{11}} & \frac{\partial V_{22}}{\partial B_{12}} & \frac{\partial V_{22}}{\partial B_{22}} \end{bmatrix} . \tag{3.8}$$

Thus, calculating the quantities $\partial V_{pq}/\partial B_{kl}$ amounts to inverting a 6×6 matrix. Next, differentiating $B = FF^T$ yields

$$\frac{\partial B_{kl}}{\partial F_{pq}} = \delta_{kp}F_{lq} + F_{kq}\delta_{lp} \ . \tag{3.9}$$

Finally, by the Chain Rule then

$$\frac{\partial V_{ij}}{\partial F_{pq}} = \frac{\partial V_{ij}}{\partial B_{kl}}\frac{\partial B_{kl}}{\partial F_{pq}} \ . \tag{3.10}$$

4. The Logarithmic Strain Tensor

The logarithmic strain ε is defined by

$$\varepsilon = \ln V \ . \tag{4.1}$$

Once again, the logarithm is calculated via the three-dimensional eigenproblem

$$V^E = \begin{bmatrix} \lambda_0 & 0 & 0 \\ 0 & \lambda_1 & 0 \\ 0 & 0 & \lambda_2 \end{bmatrix} , \quad V^E = \psi V \psi^T \ , \quad \varepsilon^E = \begin{bmatrix} \ln\lambda_0 & 0 & 0 \\ 0 & \ln\lambda_1 & 0 \\ 0 & 0 & \ln\lambda_2 \end{bmatrix} , \quad \varepsilon = \psi^T \varepsilon^E \psi \ . \tag{4.2}$$

To calculate the required gradients $\partial\varepsilon_{ij}/\partial V_{pq}$, differentiate the last of eqns. (4.2). One obtains

$$\frac{\partial \varepsilon_{ij}}{\partial V_{pq}} = \frac{\partial \varepsilon^E_{kl}}{\partial V_{pq}} \psi_{ki}\psi_{lj} + \varepsilon^E_{kl} \frac{\partial \psi_{ki}}{\partial V_{pq}} \psi_{lj} + \varepsilon^E_{kl}\psi_{ki} \frac{\partial \psi_{lj}}{\partial V_{pq}} \; , \tag{4.3}$$

where

$$\frac{\partial \varepsilon^E}{\partial V_{pq}} = \begin{bmatrix} \frac{1}{\lambda_0}\frac{\partial \lambda_0}{\partial V_{pq}} & 0 & 0 \\ 0 & \frac{1}{\lambda_1}\frac{\partial \lambda_1}{\partial V_{pq}} & 0 \\ 0 & 0 & \frac{1}{\lambda_2}\frac{\partial \lambda_2}{\partial V_{pq}} \end{bmatrix} . \tag{4.4}$$

Note that the derivatives $\partial\psi_{ij}/\partial V_{pq}$ and $\partial\lambda_i/\partial V_{pq}$ appearing in eqns. (4.3) and (4.4) are as per, respectively, eqns. (2.11) and (2.13) with V_{pq} replacing A_{pq}.

5. Example

A program was written using the formulas in Secs. 2 through 4, and as numerical example of using the formulas, consider the deformation gradient

$$F = \begin{bmatrix} 0.75 & 0.25 & 0.5 \\ -0.125 & 1.5 & -0.75 \\ -1.75 & 2.0 & 1.25 \end{bmatrix} . \tag{5.1}$$

The above-mentioned program gives for the left stretch tensor

$$V = \begin{bmatrix} 0.933\,900 & -0.027\,895\,4 & -0.045\,306\,0 \\ -0.027\,895\,4 & 1.603\,16 & 0.507\,169 \\ -0.045\,306\,0 & 0.507\,169 & 2.892\,36 \end{bmatrix} , \tag{5.2}$$

and for the logarithmic strain

$$\varepsilon = \begin{bmatrix} -0.069\,092\,3 & -0.018\,849\,2 & -0.024\,117\,6 \\ -0.018\,849\,2 & 0.437\,725 & 0.236\,368 \\ -0.024\,117\,6 & 0.236\,368 & 1.038\,92 \end{bmatrix} . \tag{5.3}$$

The results (5.2) and (5.3) have been verified by solving the two eigenproblems for V and ε by hand.