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Simultaneous pure and simple shear: the unifying deformation matrix

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ABSTRACT

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Any simultaneous combination of finite simple shear and finite pure shear is a linear transformation which can be expressed as a single transformation matrix. For two dimensions, the matrix is upper triangular with an off-diagonal term, Γ, called the effective shear strain. Γ is a simple function of the pure and simple shear components. For three dimensions, a simultaneous combination of thrusting in the x direction, thrusting in the y direction, and a wrench in the x direction, in addition to 3 orthogonal components of coaxial strain, can also be represented by a 3×3, upper triangular matrix. Here, three off-diagonal terms (Γ_{xy}, Γ_{xz}, and Γ_{yz}) occur. Γ_{xy} is a simple function of the horizontal coaxial strain values and thrusting in the x direction, Γ_{yz} depends on the coaxial strain components in the y and z directions and the thrusting in the y direction, while Γ_{xz} is related to all six strain components. The matrix also allows for volume change, either homogeneously or preferentially in a single direction. A method of decomposing the deformation matrix into a series of incremental deformation matrices, where each incremental deformation records the same kinematic vorticity number as the finite deformation is shown. The orientation and magnitude of the finite-strain ellipsoid (ellipse) is easily and accurately found at any increment during the deformation.

Introduction

There is at least two ways of thinking about plane strain deformations. One is to distinguish between the actual stretch (length of principal strain axes) and the rotation of the principal strain axes (Elliott, 1972). Another way is to consider deformation in terms of simple shear, pure shear, and/or volume change. Although these are completely equivalent, a brief literature search reveals that thinking in terms of simple and pure shear is more common, probably due to the importance of boundary conditions in geological analysis. Besides from being easy to visualize and conceive, they are the end-members of geologically realistic, two-dimensional non-spinning deformation (Lister and Williams, 1983). Since it was shown that simple shear (with or without additional anisotropic volume change) is the fundamental deformation in "perfect" shear zones (Ramsay and Graham, 1970), these terms have been used in almost any paper dealing with natural shear zones. However, most shear zones do not obey the constraints set forward by Ramsay and Graham, and pure shear and/or general volume change must be combined with simple shear to explain the observed structures. This is not straightforward if the simple shear, volume change, and pure shear were simultaneous. Since the same final deformation state can accumulate by any sequence of pure and simple shear deformation, resulting in the same finite strain ellipse and the same finite rotation and stretch of material lines, several geologists have modeled finite deformation as a

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sequence of strain superposition, e.g., simple shear followed by pure shear etc. (e.g., Ramsay, 1980; Kligfield et al., 1981; Sanderson, 1982; Coward and Potts, 1983; Sanderson and Marchini, 1984). However, incremental parameters, such as the orientation of the incremental strain ellipse or the sequence of deformation of material lines (Passchier, 1990), require the knowledge of strain history, which is demonstrably different for different sequences of strain superposition.

Ramberg (1975a,b) and several subsequent workers have approached this problem in a purely continuum mechanics framework (Means et al., 1980; McKenzie and Jackson, 1983; Means, 1983; Bobyarchick, 1986; Passchier, 1986; Weijermars, 1991). Conversely, this work uses an incremental mathematical approach to find the exact solutions and puts the results in time-independent solutions. Based on Ramberg's work, we first present a general solution to any simultaneous combination of pure and simple shear given in terms of the simple shear and coaxial strain components (with or without volume change) only. The advantage to this approach is its simplicity: any deformation can be broken up into easily conceivable geological quantities that all belong to one deformation matrix. Further, the magnitude and orientation of the finite strain ellipse can be easily calculated at any point in the deformation, without following particular particle paths.

We then show a similar solution to the three-dimensional problem of combining a coaxial deformation with up to three orthogonal simple shears, following the same method as for the two-dimensional case. Although three-dimensional deformation matrices are given by Ramberg (1975b) and McKenzie and Jackson (1983), these use instantaneous strain rates and are less general than the matrix derived in this article.

Two dimensions

Homogeneous deformation is a linear transformation which may be expressed by the general deformation (gradient) matrix **D** (cf. Flinn 1979) so that an initial particle or vector **x** is transformed into a new position **x**′ according to the transformation:

$$\mathbf{x}' = \mathbf{D}\mathbf{x}$$

If one wishes to consider the deformation in terms of simple shear (upper triangular matrix $\mathbf{D}_{ss}$) and pure shear (diagonal matrix $\mathbf{D}_{ps}$), the order by which these deformations are applied is not arbitrary, since matrix multiplication in general is non-commutative (Fig. 1):

$$\mathbf{D}_{ss}\mathbf{D}_{ps} \neq \mathbf{D}_{ps}\mathbf{D}_{ss}$$

Hence, one of two very special deformation histories, i.e. pure shear followed by simple shear, or vice versa, must be assumed if a combination of pure and simple shear is to be treated. In general, however, simple and pure shear act simultaneously during deformation. An approximate solution to this case may be found by successively multiplying small increments of simple shear and pure shear:

$$\mathbf{D} \cong \begin{bmatrix} 1 & \Delta\gamma \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 1+\Delta\epsilon_1 & 0 \\ 0 & 1+\Delta\epsilon_2 \end{bmatrix}\begin{bmatrix} 1 & \Delta\gamma \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 1+\Delta\epsilon_1 & 0 \\ 0 & 1+\Delta\epsilon_2 \end{bmatrix}\cdots\begin{bmatrix} 1 & \Delta\gamma \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 1+\Delta\epsilon_1 & 0 \\ 0 & 1+\Delta\epsilon_2 \end{bmatrix} \quad (1)$$

where $1+\epsilon_1$ and $1+\epsilon_2$ are the maximum and minimum principal extensions, respectively. This series converges to the correct path and finite strain matrix as Δ approaches zero. Ramberg (1975a) showed that, introducing the instantaneous pure shear strain rates $\dot{\epsilon} = \partial x/\partial t$, $\dot{\epsilon} = \partial y/\partial t$ and the simple shear strain rate $\dot{\gamma} = \partial\gamma/\partial t$, the particle paths for simultaneous simple and pure shear can be traced according to the formulation:

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{bmatrix} x + \dfrac{\dot{\gamma}}{2\dot{\epsilon}_x}y & \dfrac{-\dot{\gamma}}{2\dot{\epsilon}_x}y \\ 0 & y \end{bmatrix}\begin{pmatrix} \exp(\dot{\epsilon}_x t) \\ \exp(-\dot{\epsilon}_x t) \end{pmatrix} \quad (2)$$

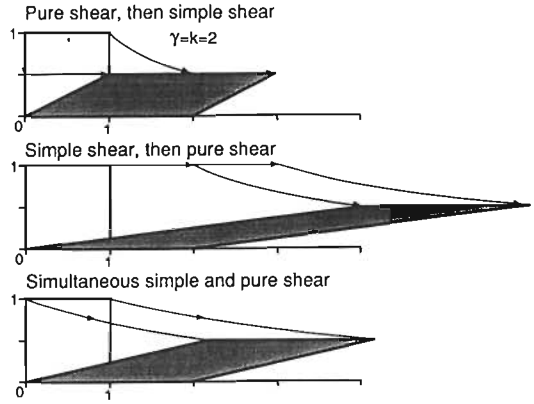

Fig. 1. The difference between discrete and simultaneous simple and pure shear, demonstrating the non-commutative nature of matrix multiplication.

which for finite deformations can be rewritten as:

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{bmatrix} \exp(\dot{\epsilon}_x t) & \dot{\gamma}\dfrac{\exp(\dot{\epsilon}_x t) - \exp(-\dot{\epsilon}_x t)}{2\dot{\epsilon}_x} \\ 0 & \exp(-\dot{\epsilon}_x t) \end{bmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \tag{3}$$

Ramberg's (1975a, p. 11) derivation can be modified to allow for volume change, in which case eq. (2) becomes:

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{bmatrix} x + \dfrac{\dot{\gamma}}{\dot{\epsilon}_x - \dot{\epsilon}_y} y & \dfrac{-\dot{\gamma}}{\dot{\epsilon}_x - \dot{\epsilon}_y} y \\ 0 & y \end{bmatrix} \begin{pmatrix} \exp(\dot{\epsilon}_x t) \\ \exp(\dot{\epsilon}_y t) \end{pmatrix} \tag{4}$$

and eq. (3) becomes:

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{bmatrix} \exp(\dot{\epsilon}_x t) & \dot{\gamma}\dfrac{\exp(\dot{\epsilon}_x t) - \exp(\dot{\epsilon}_y t)}{(\dot{\epsilon}_x - \dot{\epsilon}_y)} \\ 0 & \exp(\dot{\epsilon}_y t) \end{bmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \tag{5}$$

This transformation equation defines a time-dependent deformation matrix. This result is similar to those of McKenzie and Jackson (1983) and Weijermaars (1991), who both use slightly different approaches involving strain rates. For both the path-related and finite-strain transformation equations, we want to find expressions in terms of pure and simple shear components.

Finite strain

If the deformation matrices of pure and simple shear are written as:

$$\mathbf{D}_{\text{ps}} = \begin{bmatrix} k_1 & 0 \\ 0 & k_2 \end{bmatrix} = \begin{bmatrix} k & 0 \\ 0 & 1/k \end{bmatrix}, \qquad \mathbf{D}_{\text{ss}} = \begin{bmatrix} 1 & \gamma \\ 0 & 1 \end{bmatrix}$$

we want a single deformation matrix **D** of the form:

$$\mathbf{D}=\begin{bmatrix} k & f(\gamma,k) \\ 0 & 1/k \end{bmatrix}$$

where the off-diagonal (rotational) term is a function of both the pure and simple shear components, and may be termed Γ (effective shear strain). Hence, $k=\exp(\dot{\epsilon}_x t)$, or $\dot{\epsilon}_x=\ln(k)/t$, and $\dot{\gamma}=\gamma/t$. Substituting this expression into eq. (3) and simplifying gives the deformation matrix for simultaneous simple and pure shear:

$$\mathbf{D}=\begin{bmatrix} k & \Gamma \\ 0 & 1/k \end{bmatrix}=\begin{bmatrix} k & \dfrac{\gamma(k-1/k)}{2\ \ln\ k} \\ 0 & 1/k \end{bmatrix} \tag{6}$$

This matrix is similar to the one derived by Merle (1986).

If volume change is included in the pure shear matrix ($k_1 k_2 \neq 1$), the deformation matrix for simultaneous simple shear, pure shear, and volume change becomes:

$$\mathbf{D}=\begin{bmatrix} k_1 & \dfrac{\gamma(k_1-k_2)}{\ln\ k_1/k_2} \\ 0 & k_2 \end{bmatrix} \tag{7}$$

The function $\Gamma=\gamma(k-1/k)/2\ \ln(k)$ describes the rotational component of the deformation. Γ can easily be found by direct calculation or by using the graph of Γ/γ against k, shown in Figure 2. Note that a deformation that involves shear along the y axis and, therefore has a related deformation matrix of the form:

$$\mathbf{D}=\begin{bmatrix} k & 0 \\ \Gamma & 1/k \end{bmatrix} \tag{8}$$

which is symmetric to the problem discussed above. The two deformation matrices, eqs. (6) and (8), become equal if the x and y axes are switched. The value and orientation of the principal elongations, the volume change, and the rotational component of the deformation can now easily be extracted from the deformation matrix in eq. (7) (see Appendix 1).

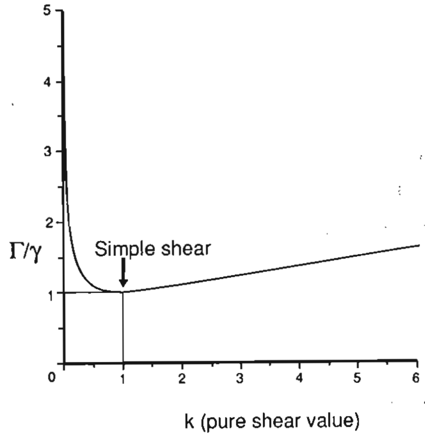

Fig. 2. A plot of Γ (the effective shear strain) / γ (simple shear strain) versus k (pure shear component). At $k=1$ (simple shear), $\Gamma/\gamma=1$. At $k\neq 1$, the effective shear strain becomes larger than just the simple shear component of deformation. This effect increases as k is farther removed from 1, either toward zero or infinity.

A mathematical consequence of this derivation is that k in eq. (6) may not be set exactly to one, because the $\ln(k)$ term in the denominator and the $(k - 1/k)$ term in the numerator of Γ both become zero, in the case of no volume change. Similarly, k_1 may not equal k_2 in eq. (7). These problems can be resolved by setting k (or k_1) slightly different from 1 (or k_2), say 1.00001. Since $k = 1$ corresponds to a simple shearing deformation history, one can use the simplified matrices given in Appendix 2.

Strain paths

To investigate the strain path in terms of pure and simple shear, one can choose a fixed strain increment and calculate the deformation matrix after each increment (Elliott, 1972). For n increments and a constant pure shear/simple shear ratio throughout deformation, the incremental simple shear (γ_{incr}) simply becomes $(\gamma_{\text{total}})/n$, and k_{incr} becomes $(k_{\text{total}})^{(1/n)}$. The incremental deformation matrix can be written as:

$$\mathbf{D}_{\text{incr}} = \begin{bmatrix} k_{\text{incr}} & \Gamma_{\text{incr}} \\ 0 & 1/k_{\text{incr}} \end{bmatrix} = \begin{bmatrix} (k_{\text{total}})^{1/n} & n^{-1}\gamma_{\text{total}} \dfrac{(k_{\text{total}})^{1/n} - 1/(k_{\text{total}})^{1/n}}{2\ln(k_{\text{total}})^{1/n}} \\ 0 & 1/(k_{\text{total}})^{1/n} \end{bmatrix} \tag{9}$$

Note that $\Gamma_{\text{incr}} \neq (\Gamma_{\text{total}})/n$ and $\Gamma_{\text{incr}} \neq (\Gamma_{\text{total}})^{(1/n)}$ due to its dependence on both k and γ. The matrix (9) gives the exact incremental strain for any steady state, or constant kinematic vorticity number, combination of pure and simple shear. The relationship between the incremental and finite deformation matrices is:

$$\mathbf{D}_{\text{total}} = \begin{bmatrix} k_{\text{total}} & \Gamma_{\text{total}} \\ 0 & k_{\text{total}} \end{bmatrix} = \begin{bmatrix} k_{\text{incr}} & \Gamma_{\text{incr}} \\ 0 & 1/k_{\text{incr}} \end{bmatrix}^n \tag{10}$$

and the deformation matrix after, say, three increments is:

$$\begin{bmatrix} k & \Gamma \\ 0 & 1/k \end{bmatrix}_{\text{3increments}} = \begin{bmatrix} k & \Gamma \\ 0 & 1/k \end{bmatrix}_{\text{incr}} \begin{bmatrix} k & \Gamma \\ 0 & 1/k \end{bmatrix}_{\text{incr}} \begin{bmatrix} k & \Gamma \\ 0 & 1/k \end{bmatrix}_{\text{incr}}$$

The orientation, magnitudes, and rotation of the principal strains can be calculated at any step (see Appendix 1) and thus mapped throughout the deformation.

Kinematic vorticity number

Recent workers have used the kinematic vorticity number, W_k, to define the relative amounts of pure and simple shear in a single deformation (Means et al., 1980; Passchier, 1986; Bobyarchick, 1986). The kinematic vorticity is defined by Trusdell (1953) as:

$$W_k = \frac{w}{\sqrt{2(S_1^2 + S_2^2 + S_3^2)}} \tag{11}$$

where w is the magnitude of the vorticity vector and S_i are the principal strain rates (also see Means et al., 1980). Again, we choose to relate kinematic vorticity to the pure and simple shear components of deformation. Bobyarchick (1986), using a Mohr-circle construction, defines the kinematic vorticity number in terms of the instantaneous pure shear strain rate, $\dot{\epsilon}_x$, and the simple shear strain rate, $\dot{\gamma}$:

$$W_k = \cos[\arctan(2\dot{\epsilon}_x/\dot{\gamma})]$$

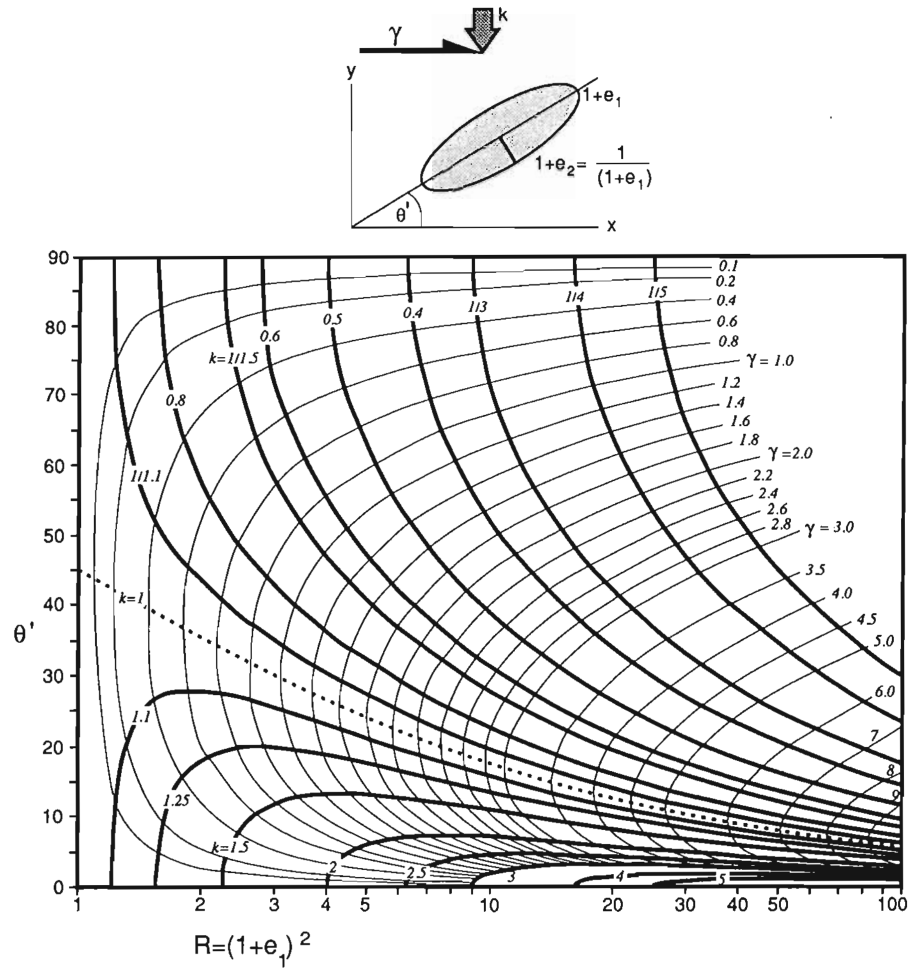

Fig. 3. R-θ'diagram where θ' is the angle between the shear plane (zone) and the long axis of the finite-strain ellipse, and R is the strain axes ratio. This graph is for simultaneous simple and pure shear, and is similar to that shown by Merle (1986). The thin lines show constant simple shear (γ) values, while the thick lines show constant pure shear (k).

Substituting $k = \exp(\dot{\epsilon}_x t)$, or $\dot{\epsilon}_x = \ln(k)/t$, and $\dot{\gamma} = \gamma/t$ into eq. (11) and simplifying, we arrive at the result:

$$W_k = \cos\{\arctan[2\ \ln(k)/\gamma]\} \tag{12}$$

This result includes the conditions of $W_k = 1$, implying simple shear, and $W_k = 0$ implying pure shear. The effect of various combinations of simple and pure shear on the rotation and displacement during deformation may be extracted from the matrix in eq. (6), as is illustrated in Figure 3.

It can be shown that a deformation can be divided into any number of incremental steps, in the manner shown above, all of which have the same W_k value. For any increment of deformation, W_k is given by the relationship:

$$W_k = \cos\{\arctan[2\ \ln(k_{\text{incr}})/\gamma_{\text{incr}}]\} \tag{13}$$

As noted above, there is a straightforward relationship between the incremental and total deformation, such that $\gamma_{\text{incr}} = \gamma_{\text{total}}/n$, and $k_{\text{incr}} = k_{\text{total}}^{(1/n)}$. Substiting these values into eq. (13), we get:

$$W_k = \cos\{\arctan[2\ \ln(k_{\text{total}}^{(1/n)})/(\gamma_{\text{total}}/n)]\} \tag{14}$$

Using the relationship ln $(a^b) = b \ln a$, for the numerator, the kinematic voriticity is:

$$W_k = \cos\{\arctan[(2/n)\ \ln(k_{\text{total}})/(\gamma_{\text{total}}/n)]\} = \cos[\arctan(2\ \ln(k_{\text{total}})/\gamma_{\text{total}})] \quad (15)$$

Since n, the number of increments, cancels in the numerator and denominator, there is no dependence of W_k on the number of increments. Therefore, W_k is the same for all increments of deformation, as well as the final deformation state.

General two-dimensional deformation

The deformation matrix, given in eq. (7), is only applicable for simple shear orthogonal to the pure shear and/or volume loss components of deformation. A general deformation matrix would allow simple shear at an inclined angle to the pure shear components. Using the same method as above, a solution to the general, two-dimensional deformation matrix is given in terms of instantaneous pure shear and simple shear rates, and inclination, θ, of the simple shear plane to the coaxial strain components (eqs. 46–49 of Ramberg, 1975a). However, as with the case of a simple shear component orthogonal to the pure shear components, we would like the deformation in terms of pure shear and simple shear components only. Using the relationships $\dot{\epsilon}_x = \ln(k_1)/t$, $\dot{\epsilon}_y = \ln(k_2)/t$, and $\dot{\gamma} = \gamma/t$, substituting into Ramberg's equations, and generalizing to include volume loss, we arrive at a time-independent deformation matrix of the form:

$$\mathbf{D} = \begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{bmatrix}$$

where the components are given by:

$$D_{11} = \frac{(\chi_2 - a_{11})\ \exp(\chi_1) + (a_{11} - \chi_1)\ \exp(\chi_2)}{\chi_2 - \chi_1} \quad (16a)$$

$$D_{12} = \frac{a_{12}(\exp(\chi_2) - \exp(\chi_1))}{\chi_2 - \chi_1} \quad (16b)$$

$$D_{21} = \frac{a_{21}(\exp(\chi_2) - \exp(\chi_1))}{\chi_2 - \chi_1} \quad (16c)$$

and

$$D_{22} = \frac{(\chi_2 - a_{22})\ \exp(\chi_1) + (a_{22} - \chi_1)\ \exp(\chi_2)}{\chi_2 - \chi_1} \quad (16d)$$

The eigenvalue χ is given by:

$$\chi_i = \tfrac{1}{2}(a_{11} + a_{22}) \pm \tfrac{1}{2}\left[(a_{11} + a_{22})^2 + 4a_{12}a_{21}\right]^{1/2} \quad (17)$$

and

$$a_{11} = \ln k_1 - \gamma \sin\theta \cos\theta \quad (18a)$$

$$a_{12} = \gamma \cos^2\theta \quad (18b)$$

$$a_{21} = -\gamma \sin^2\theta \quad (18c)$$

and

$$a_{22} = \ln k_2 + \gamma \sin \theta \cos \theta \tag{18d}$$

This approach can be used to model complex geological situations, such as strain accumulations on the limbs of folds (Ramberg, 1975a) or volume change, perhaps in the form of cleavage development, occurring at an inclined angle to the shear plane. The finite-strain ellipse and kinematic vorticity for the deformation matrix can be found by using the methods outlined in Appendix 1 and the previous section, respectively.

Three dimensions

In three dimensions, we would like the finite deformation matrix to be written as:

$$\mathbf{D} = \begin{bmatrix} k_1 & \Gamma_{xy} & \Gamma_{xz} \\ 0 & k_2 & \Gamma_{yz} \\ 0 & 0 & k_3 \end{bmatrix} \tag{19}$$

where the k_1, k_2, and k_3 represent extensions along the x, y, and z coordinate axes, respectively, and the off-diagonal terms represent elements of effective shear deformation. We consider a left-handed coordinate system with the z axis vertical. The subscript refers to the principal deformation plane, the plane in which the most shearing occurs and which is orthogonal to the shear plane. The first character in the subscript indicates the shear direction. Further, the intersection of the principal deformation plane and the shear plane is the shear direction. The deformation described in eq. (19) consists of simultaneous thrusting in the x direction (Γ_{xz}), thrusting in the y direction (Γ_{yz}), wrenching in the x direction (Γ_{xy}), coaxial strain, and/or volume change. These deformation components are shown in Figure 4. Since most macro- and mesoscopic geological modeling is normally confined to one or two simultaneous shear systems, combined with coaxial strain and/or volume change, this relatively general combination covers a number of realistic deformations in the crust.

In three dimensions, the order of deformation is slightly more complicated than the two-dimensional case. Some combinations of orthogonal simple shears are commutative, i.e. the strain history does not influence the finite deformation. The following combinations are commutative:

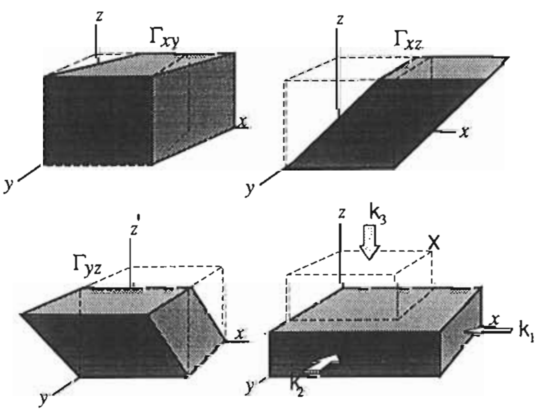

Fig. 4. A diagram of the various types of deformation described by the upper triangular matrix in eq. (19). The resulting deformation matrix, eq. (30), can describe the simultaneous result of all these deformations.

(1) combination of Γ_{xy} and Γ_{xz}
(2) combination of Γ_{xz} and Γ_{yz}.

For these two cases, the order of matrix multiplication (strain history) is of no importance, as can be illustrated for case 1:

$$\mathbf{D}=\begin{bmatrix}1 & \Gamma_{xy} & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{bmatrix}\begin{bmatrix}1 & 0 & \Gamma_{xz}\\ 0 & 1 & 0\\ 0 & 0 & 1\end{bmatrix}=\begin{bmatrix}1 & 0 & \Gamma_{xz}\\ 0 & 1 & 0\\ 0 & 0 & 1\end{bmatrix}\begin{bmatrix}1 & \Gamma_{xy} & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{bmatrix}=\begin{bmatrix}1 & \Gamma_{xy} & \Gamma_{xz}\\ 0 & 1 & 0\\ 0 & 0 & 1\end{bmatrix} \tag{20}$$

Also, a simple shear combined with an uniaxial lengthening or shortening perpendicular, but only perpendicular, to the shear plane, is history independent. For example, a $k_1 \neq 1$ combined with a Γ_{yz} is independent of strain history:

$$\mathbf{D}=\begin{bmatrix}k_1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{bmatrix}\begin{bmatrix}1 & 0 & 0\\ 0 & 1 & \Gamma_{xy}\\ 0 & 0 & 1\end{bmatrix}=\begin{bmatrix}1 & 0 & 0\\ 0 & 1 & \Gamma_{xy}\\ 0 & 0 & 1\end{bmatrix}\begin{bmatrix}k_1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{bmatrix}=\begin{bmatrix}k_1 & 0 & 0\\ 0 & 1 & \Gamma_{xy}\\ 0 & 0 & 1\end{bmatrix}$$

Any other combination of the strain components of matrix (19) is non-commutative, and a single deformation matrix for their simultaneous operation is not simply the product of the individual deformation matrices. However, a single matrix for the combination of one or more orthogonal shears, combined with coaxial strain and/or volume change, can be found. For simplicity, the coaxial strain axes are taken to be perpendicular to the shear planes.

Expanding the analysis of Ramberg (1975a) to three dimensions, the transformation is, in terms of the instantaneous strain rates:

$$\begin{pmatrix}\dot{x}\\ \dot{y}\\ \dot{z}\end{pmatrix}=\begin{bmatrix}\dot{\epsilon}_1 & \dot{\gamma}_{xy} & \dot{\gamma}_{xz}\\ 0 & \dot{\epsilon}_2 & \dot{\gamma}_{yz}\\ 0 & 0 & \dot{\epsilon}_3\end{bmatrix}\begin{pmatrix}x'\\ y'\\ z'\end{pmatrix} \tag{21}$$

Here, $\dot{x}=\partial x/\partial t$, $\dot{y}=\partial y/\partial t$, and $\dot{z}=\partial z/\partial t$. Assuming that the strain rates stay constant with time, and that the strain is homogeneous, the system has a solution of the form:

$$\begin{pmatrix}x'\\ y'\\ z'\end{pmatrix}=\begin{bmatrix}c_{11} & c_{12} & c_{13}\\ c_{21} & c_{22} & c_{23}\\ c_{31} & c_{32} & c_{33}\end{bmatrix}\begin{pmatrix}\exp(\dot{\epsilon}_x t)\\ \exp(\dot{\epsilon}_y t)\\ \exp(\dot{\epsilon}_z t)\end{pmatrix} \tag{22}$$

To find the coefficient matrix, we first set $t=0$ so that the exponential vector becomes (1, 1, 1), and obtain the relationship:

$$\begin{bmatrix}c_{11}+c_{12}+c_{13}\\ c_{21}+c_{22}+c_{23}\\ c_{31}+c_{32}+c_{32}\end{bmatrix}=\begin{pmatrix}x'\\ y'\\ z'\end{pmatrix} \tag{23}$$

Six more equations are required to solve for the coefficients. From the theory of differential equations, we note that the column vectors (c_{11}, c_{21}, c_{31}), (c_{12}, c_{22}, c_{32}), and (c_{13}, c_{23}, c_{33}) in the coefficient matrix in (22) are the eigenvectors of the matrix in eq. (21). This gives us three systems of equations. For the first eigenvector, we get:

$$\begin{bmatrix}\dot{\epsilon}_1 & \dot{\gamma}_{xy} & \dot{\gamma}_{xz}\\ 0 & \dot{\epsilon}_2 & \dot{\gamma}_{yz}\\ 0 & 0 & \dot{\epsilon}_3\end{bmatrix}\begin{pmatrix}c_{11}\\ c_{21}\\ c_{31}\end{pmatrix}=\dot{\epsilon}_x\begin{pmatrix}c_{11}\\ c_{21}\\ c_{31}\end{pmatrix}$$

or:

$$\begin{bmatrix} \dot{\epsilon}_x c_{11} + \gamma_{xy} c_{21} + \gamma_{yz} c_{31} \\ \dot{\epsilon}_y c_{21} + \gamma_{yz} c_{31} \\ \dot{\epsilon}_y c_{31} \end{bmatrix} = \begin{pmatrix} \dot{\epsilon}_x c_{11} \\ \dot{\epsilon}_x c_{21} \\ \dot{\epsilon}_x c_{31} \end{pmatrix} \tag{24}$$

For the other eigenvectors, we get:

$$\begin{bmatrix} \dot{\epsilon}_x c_{12} + \gamma_{xy} c_{22} + \gamma_{yz} c_{32} \\ \dot{\epsilon}_y c_{22} + \gamma_{yz} c_{32} \\ \dot{\epsilon}_y c_{32} \end{bmatrix} = \begin{pmatrix} \dot{\epsilon}_y c_{12} \\ \dot{\epsilon}_{y22} \\ \dot{\epsilon}_y c_{32} \end{pmatrix} \tag{25}$$

and:

$$\begin{bmatrix} \dot{\epsilon}_x c_{13} + \gamma_{xy} c_{23} + \gamma_{yz} c_{33} \\ \dot{\epsilon}_y c_{23} + \gamma_{yz} c_{33} \\ \dot{\epsilon}_y c_{33} \end{bmatrix} = \begin{pmatrix} \dot{\epsilon}_z c_{13} \\ \dot{\epsilon}_z c_{23} \\ \dot{\epsilon}_z c_{33} \end{pmatrix} \tag{26}$$

Combining eqs. (23), (24), (25), and (26), and simplifying gives:

$$c_{21} = c_{31} = c_{32} = 0$$

$$c_{11} = x + \frac{\gamma_{xy} y}{\dot{\epsilon}_x - \dot{\epsilon}_y} + \frac{\gamma_{xy}\gamma_{yz} z}{(\dot{\epsilon}_x - \dot{\epsilon}_y)(\dot{\epsilon}_y - \dot{\epsilon}_z)} - \frac{\gamma_{xy}\gamma_{yz} z}{(\dot{\epsilon}_y - \dot{\epsilon}_z)(\dot{\epsilon}_x - \dot{\epsilon}_z)} + \frac{\gamma_{xz} z}{\dot{\epsilon}_x - \dot{\epsilon}_z}$$

$$c_{12} = \frac{-\gamma_{xy} y}{\dot{\epsilon}_x - \dot{\epsilon}_y} - \frac{\gamma_{xy}\gamma_{yz} z}{(\dot{\epsilon}_x - \dot{\epsilon}_y)(\dot{\epsilon}_y - \dot{\epsilon}_z)}$$

$$c_{13} = \frac{\gamma_{xy}\gamma_{yz} z}{(\dot{\epsilon}_y - \dot{\epsilon}_z)(\dot{\epsilon}_x - \dot{\epsilon}_z)} - \frac{\gamma_{xz} z}{\dot{\epsilon}_x - \dot{\epsilon}_z}$$

$$c_{22} = y + \frac{\gamma_{yz}}{\dot{\epsilon}_y - \dot{\epsilon}_z} z$$

$$c_{23} = \frac{-\gamma_{yz}}{\dot{\epsilon}_y - \dot{\epsilon}_z} z$$

$$c_{33} = z$$

We now insert these coefficients into eq. (22) to get a particle path equation:

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = C \begin{pmatrix} \exp(\dot{\epsilon}_x t) \\ \exp(\dot{\epsilon}_y t) \\ \exp(\dot{\epsilon}_z t) \end{pmatrix} \tag{27}$$

where **C** is given by the matrix:

$$C = \begin{bmatrix} c_{11} & c_{12} & c_{13} \\ 0 & c_{22} & c_{23} \\ 0 & 0 & c_{33} \end{bmatrix}$$

This equation corresponds to the two-dimensional eq. (4). For finite deformations, we can rewrite eq. (21) to obtain the time and strain rate-dependent deformation matrix:

$$\mathbf{D}=\begin{bmatrix} \exp(\dot{\epsilon}_{xt}) & \dfrac{\dot{\gamma}_{xy}A}{(\dot{\epsilon}_x-\dot{\epsilon}_y)} & \dfrac{\dot{\gamma}_{yz}\gamma_{xy}A}{(\dot{\epsilon}_x-\dot{\epsilon}_y)(\dot{\epsilon}_y-\dot{\epsilon}_z)}+\dfrac{\dot{\gamma}_{yz}\dot{\gamma}_{xy}B}{(\dot{\epsilon}_y-\dot{\epsilon}_z)(\dot{\epsilon}_x-\dot{\epsilon}_z)}+\dfrac{-\dot{\gamma}_{xz}B}{(\dot{\epsilon}_x-\dot{\epsilon}_z)} \\ 0 & \exp(\dot{\epsilon}_y t) & \dfrac{\dot{\gamma}_{yz}C}{(\dot{\epsilon}_y-\dot{\epsilon}_z)} \\ 0 & 0 & \exp(\dot{\epsilon}_z t) \end{bmatrix} \tag{28}$$

where $A=\{\exp(\dot{\epsilon}_x t)-\exp(\dot{\epsilon}_y t)\}$, $B=\{\exp(\dot{\epsilon}_z t)-\exp(\dot{\epsilon}_x t)\}$, and $C=\{\exp(\dot{\epsilon}_y t)-\exp(\dot{\epsilon}_z t)\}$, which relates the undeformed to the deformed state. Hence, we have the relationship $\mathbf{x}'=\mathbf{D}\mathbf{x}$. This matrix (**D**) corresponds to the two-dimensional matrix in eq. (5) above.

We now want to express the deformation matrix **D** in terms of coaxial deformation components (k_1, k_2, and k_3) and simple shear components (γ_{xz}, γ_{yz}, and γ_{xy}), as in eq. (19). Comparing this with the matrix in (28), we get:

$$\dot{\gamma}_{xz}=\gamma_{xz}/t,\quad \dot{\gamma}_{yz}=\gamma_{yz}/t,\quad \dot{\gamma}_{xy}=\gamma_{xy}/t,$$

and:

$$\exp(\dot{\epsilon}_x t)=k_1,\quad \exp(\dot{\epsilon}_y t)=k_2,\quad \exp(\dot{\epsilon}_z t)=k_3,$$

and for unit time:

$$\dot{\epsilon}_x=\ln k_1,\quad \dot{\epsilon}_y=\ln k_2,\quad \dot{\epsilon}_z=\ln k_3,\quad \dot{\gamma}_{xz}=\gamma_{xz},\quad \dot{\gamma}_{yz}=\gamma_{yz},\quad \dot{\gamma}_{xy}=\gamma_{xy}. \tag{29}$$

Inserting these relationships into matrix (28) and simplifying gives the deformation matrix:

$$\mathbf{D}=\begin{bmatrix} k_1 & \dfrac{\gamma_{xy}(k_1-k_2)}{\ln(k_1/k_2)} & \dfrac{\gamma_{xz}(k_1-k_3)}{\ln(k_1/k_3)}+\dfrac{\gamma_{yz}\gamma_{xy}(k_1-k_2)}{\ln(k_1/k_2)\ln(k_2/k_3)}+\dfrac{\gamma_{yz}\gamma_{xy}(k_3-k_1)}{\ln(k_2/k_3)\ln(k_1/k_3)} \\ 0 & k_2 & \dfrac{\gamma_{yz}(k_2-k_3)}{\ln(k_2/k_3)} \\ 0 & 0 & k_3 \end{bmatrix}. \tag{30}$$

Using eq. (30), the geometry and orientation of the strain ellipsoid can be determined at any point in the deformation history, by solving for the eigenvalues and eigenvectors of $\mathbf{DD}^{\mathrm{T}}$, as illustrated for two dimensions in Appendix 1. The strain path can be solved for in the *xy*, *yz*, or *xz* planes, as demonstrated for the two-dimensional cases, eqs. (9) and (10). As with the two- dimensional case, the k values may not be set equal to each other, because of the ln terms in the denominator and (k_i-k_j) terms in the numerator of the off-diagonal positions. Since these cases are of geological importance, e.g., simple shears acting without coaxial strain components, their exact solutions are given in Appendix 2.

The general deformation matrix (30) is clearly not restricted to combinations of thrusting in the x and y directions, and wrenching in the y direction, in addition to the general coaxial strain and/or volume change. By switching the orientations of x and y, one gets a combination of thrusting and wrenching in the original y direction, and thrusting in the original x direction. Switching x and z (making x vertical) gives a combination of two vertical shears, and wrenching in the original y direction. Making y the vertical direction gives wrenching and thrusting in the initial x direction, and vertical shear in the original *xz* plane. Hence, the exact deformation matrix for a large variety of complex deformations can be found using the matrix above (30). Other combinations of simple shears, coaxial strain, and volume change can be solved for, following the procedure outlined above.

The complete deformation matrix is not needed for every deformation history. For example, a transpressional/transtensional deformation may be defined as the combination of a simultaneous simple shear in the *xy* shear plane and a pure shear in the *yz* plane (Sanderson and Marchini, 1984). Using eq. (30), one can set γ_{xz} and γ_{yz} to zero, and $k_1 = 1$ and $k_3 = 1/k_2$. The resulting deformation matrix for transpression/transtension, therefore becomes:

$$\mathbf{D} = \begin{bmatrix} 1 & \dfrac{\gamma(1-k_2)}{\ln(1/k_2)} & 0 \\ 0 & k_2 & 0 \\ 0 & 0 & 1/k_2 \end{bmatrix} \tag{31}$$

From this matrix, the precise orientations and magnitude of the principal strains can be calculated for incremental and finite strains, as can the correct angular relationships involved in the deformation (Fossen and Tikoff, in press). Note that these results differ from the formulas given by Sanderson and Marchini (1984), who used a deformation matrix that mathematically corresponds to pure shear followed by simple shear.

Another example is a combination of three-dimensional coaxial strain (e.g., general flattening/ constriction) and thrusting (horizontal simple shear) in the *x* direction. For this case, γ_{xy} and γ_{yz} become zero, and eq. (30) simplifies to:

$$\mathbf{D} = \begin{bmatrix} k_1 & 0 & \dfrac{\gamma(k_1-k_3)}{\ln(k_1/k_3)} \\ 0 & k_2 & 0 \\ 0 & 0 & k_3 \end{bmatrix} \tag{32}$$

As discussed for two dimensions, a general three-dimensional matrix can be found which allows a simultaneously acting simple shear plane inclined to all three axes of the coaxial strain components. Although this general matrix is computationally complex and difficult to apply to geological deformations, it can be determined, as well as the corresponding finite-strain ellipse and kinematic vorticity number, using the methods outlined in this paper.

Kinematic vorticity number in three dimensions

Assuming steady-state flow (eigen-flow of Passchier, 1990) and using eq. (11), we can define the kinematic vorticity in three dimensions. The velocity field for the three-dimensional deformation considered in this paper is given by eq. (21):

$$\mathbf{v} = \mathbf{Lx} \tag{33}$$

where **L** is the velocity gradient tensor. **L**, in turn, can be decomposed into $\dot{\mathbf{S}}$, the symmetric stretching tensor, and **W**, the skew-symmetric vorticity tensor (Malvern, 1969, Bobyarchick, 1986), as such:

$$\mathbf{L} = \dot{\mathbf{S}} + \mathbf{W} \tag{34}$$

Writing out the velocity field in equation form from eq. (34), we get:

$$\begin{aligned} v_1 &= \dot{\epsilon}_x x + \dot{\gamma}_{xy} y + \dot{\gamma}_{xz} z \\ v_2 &= \dot{\epsilon}_y y + \dot{\gamma}_{yz} z \\ v_3 &= \dot{\epsilon}_z z \end{aligned} \tag{35}$$

The vorticity vector **w** is defined as the curl of the velocity field **v**. Therefore, for our three-dimensional deformation, the vorticity vector is:

$$\mathbf{w} = \begin{pmatrix} \dot{\gamma}_{yz} \\ -\dot{\gamma}_{xz} \\ \dot{\gamma}_{xy} \end{pmatrix} \tag{36}$$

and its magnitude is, therefore:

$$w = \sqrt{(\dot{\gamma}_{yz})^2 + (\dot{\gamma}_{xz})^2 + (\dot{\gamma}_{xy})^2} \tag{37}$$

To find the principal strain rates, we follow the analysis of Means et al. (1980), who define the kinematic vorticity number as:

$$W_k = \frac{2}{\sqrt{2(S_1^2 + S_2^2 + S_3^2)}} = \frac{w}{\sqrt{2\overline{\Pi}}} \tag{38}$$

where $\overline{\Pi}$ is the invariant second moment of the stretching tensor. Knowing the stretching tensor:

$$\dot{\mathbf{S}} = \begin{bmatrix} \dot{\epsilon}_x & \frac{1}{2}\dot{\gamma}_{xy}^{x} & \frac{1}{2}\dot{\gamma}_{xz}^{x} \\ \frac{1}{2}\dot{\gamma}_{xy}^{x} & \dot{\epsilon}_y & \frac{1}{2}\dot{\gamma}_{yz}^{y} \\ \frac{1}{2}\dot{\gamma}_{xz}^{x} & \frac{1}{2}\dot{\gamma}_{yz}^{y} & \dot{\epsilon}_z \end{bmatrix} \tag{39}$$

we can find $\overline{\Pi}$ from the relationship (Means et al., 1980):

$$\overline{\Pi} = \mathrm{trace}(\dot{\mathbf{S}}\dot{\mathbf{S}}^{\mathrm{T}}) = \dot{\epsilon}_x^2 + \dot{\epsilon}_y^2 + \dot{\epsilon}_z^2 + \tfrac{1}{2}\left[(\dot{\gamma}_{xy})^2 + (\dot{\gamma}_{xz})^2 + (\dot{\gamma}_{yz})^2\right] \tag{40}$$

The kinematic vorticity number can thus be written as:

$$W_k = \frac{\sqrt{(\dot{\gamma}_{yz})^2 + (\dot{\gamma}_{xz})^2 + (\dot{\gamma}_{xy})^2}}{\sqrt{2(\dot{\epsilon}_x^2 + \dot{\epsilon}_y^2 + \dot{\epsilon}_z^2) + (\dot{\gamma}_{xy})^2 + (\dot{\gamma}_{xz})^2 + (\dot{\gamma}_{yz})^2}} \tag{41}$$

To relate this number to the actual components of pure and simple shear, we use the substitutions of (29) and obtain:

$$W_k = \frac{\sqrt{(\gamma_{yz})^2 + (\gamma_{xz})^2 + (\gamma_{xy})^2}}{\sqrt{2\left[\ln(k_1)^2 + \ln(k_2)^2 + \ln(k_3)^2\right] + (\gamma_{xy})^2 + (\gamma_{xz})^2 + (\gamma_{yz})^2}} \tag{42}$$

In two dimensions, this reduces to:

$$W_k = \frac{\gamma}{\sqrt{2\left[\ln(k_1)^2 + \ln(k_2)^2\right] + (\gamma)^2}} \tag{43}$$

which is equivalent to eq. (12), albeit in a different form.

To find the flow apophyses (cf. Bobyarchick, 1986) of this three-dimensional deformation, one must merely find the eigenvectors to the velocity gradient tensor **L**. The eigenvalues of **L** are simply $\dot{\epsilon}_x$, $\dot{\epsilon}_y$, and $\dot{\epsilon}_z$, and the corresponding eigenvectors can be shown to be:

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} \dfrac{-\dot{\gamma}_{xy}}{\dot{\epsilon}_x - \dot{\epsilon}_y} \\ 1 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} \dfrac{\dot{\gamma}_{xz}}{\dot{\epsilon}_x - \dot{\epsilon}_z} + \dfrac{\dot{\gamma}_{xy}\dot{\gamma}_{yz}}{(\dot{\epsilon}_x - \dot{\epsilon}_z)(\dot{\epsilon}_y - \dot{\epsilon}_z)} \\ \dfrac{-\dot{\gamma}_{yz}}{\dot{\epsilon}_y - \dot{\epsilon}_z} \\ 1 \end{pmatrix} \tag{44}$$

or, in terms of simple shear and coaxial strain components:

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \dfrac{-\gamma_{xy}}{\ln(k_1/k_2)} \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} \dfrac{\gamma_{xz}}{\ln(k_1/k_3)} + \dfrac{\gamma_{xy}\gamma_{yz}}{\ln(k_1/k_3)\ln(k_2/k_3)} \\ \dfrac{-\gamma_{yz}}{\ln(k_2/k_3)} \\ 1 \end{pmatrix} \tag{45}$$

In the absence of any simple shears, these eigenvectors reduce to the x, y, and z axes for the instantaneous directions of maximum stretching. For plane strain, one flow apophysis is parallel to the larger of the coaxial strain components (k_1 if $k_1 > k_2$), and the other is oblique to the x axis at an angle of:

$$\theta' = \arctan(y/x) = \arctan\left(\frac{\dot{\epsilon}_x - \dot{\epsilon}_y}{-\dot{\gamma}_{xy}}\right) = \arctan\left(\frac{\ln k_1 - \ln k_2}{-\gamma_{xy}}\right) \tag{46}$$

which is the same relationship as that derived by Bobyarchick (1986) using a Mohr-circle construction.

Conclusions

A method of simultaneously combining simple shear(s), coaxial strain, and/or volume change is presented. The result is in the form of a deformation matrix, moving a material point or vector from an initial, undeformed position to a final, deformed one. The deformation matrix is given only in terms of shortening (or extension) components and shear strain components, and is therefore easily applicable to geological settings. Further, the direction and magnitude of the strain ellipsoid (ellipse) are attainable at any stage during the deformation. Because simultaneous strains can be added in increments of any size, the deformation matrix derived here is also applicable to forward modeling of geological processes. During the latter case, the contribution of each deformation component can be changed during deformation, and an infinite number of deformation paths can be modeled.

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Appendix 1

The deformation matrix (incremental or final) contains complete information about the deformation, i.e. the rotation and volume (or area) change, and the length and orientation of the principal axes of the finite strain ellipsoid (ellipse). The principal elongations ($1+\epsilon_1$, $1+\epsilon_2$, and $1+\epsilon_3$) are the square roots of the eigenvalues of the matrix $\mathbf{DD}^{\mathrm{T}}$, and their orientations are given by their corresponding eigenvectors. For instance, for a given plane strain deformation $\mathbf{D}$:

$$\mathbf{D} = \begin{bmatrix} k_1 & \Gamma \\ 0 & k_2 \end{bmatrix} \tag{A1}$$

one can easily calculate $\mathbf{D}^{\mathrm{T}}$, and multiply by the original deformation matrix, to get:

$$\mathbf{D}\mathbf{D}^{T}=\begin{bmatrix}\Gamma^2+k_1^2 & k_2\Gamma\\ k_2\Gamma & k_2^2\end{bmatrix} \tag{A2}$$

The magnitudes of the principal axes of the finite strain ellipse, the eigenvalues of matrix (7), are then given by the equation:

$$\lambda=\frac{(\Gamma^2+k_1^2+k_2^2)\pm\sqrt{(\Gamma^2+k_1^2+k_2^2)^2-4k_1^2k_2^2}}{2} \tag{A3}$$

The eigenvectors, the orientation of the principal axis of the finite strain ellipse, can be found by inserting the eigenvalues into the deformation matrix. The eigenvalues must satisfy the equation:

$$(\mathbf{D}\mathbf{D}^{T}-\lambda_{\max}\mathbf{I})\mathbf{e}=\begin{bmatrix}(\Gamma^2+k_1^2)-\lambda_{\max} & k_2\Gamma\\ k_2\Gamma & k_2^2-\lambda_{\max}\end{bmatrix}\begin{bmatrix}x\\ y\end{bmatrix}=0 \tag{A4}$$

where $\mathbf{e}$ is an eigenvector. We can restrict our interest only to $\lambda_{\max}$, since we only need to know the orientation of the long axis of the finite-strain ellipse. Multiplying out eq. (A4), we get:

$$(\Gamma^2+k_1^2-\lambda_{\max})x+\Gamma k_2 y=0 \tag{A5}$$

and:

$$\Gamma k_2 x+(k_2^2-\lambda_{\max})y=0 \tag{A6}$$

Using eq. (A5), and knowing $\tan\theta'=y/x$, the angle between the long axis of the finite-strain ellipse (corresponding to the largest eigenvalue) and the positive x axis is:

$$\theta'=\arctan\left(\frac{(\Gamma^2+k_1^2-\lambda_{\max})}{-k_2\Gamma}\right) \tag{A7}$$

Although eigenvalues can be found analytically, it is more practical to substitute values into the deformation matrix and solve numerically, especially for the three-dimensional case. Notice that the finite-strain ellipse orientation is given completely in terms of k and γ values.

The fractional volume change involved equals $\det(\mathbf{D})-1$, and is negative for volume decrease, and positive for volume increase. To find the rotational component of the deformation the matrix $\mathbf{D}$ may be resolved by left polar decomposition into a "pure shear matrix" $\mathbf{T}$ and a rotational matrix $\mathbf{R}$ so that $\mathbf{D}=\mathbf{TR}$ (Elliott, 1972). The matrices are defined as:

$$\mathbf{T}=\begin{bmatrix}T_{\mathrm{I}} & 0\\ 0 & T_{\mathrm{II}}\end{bmatrix}, \tag{A8}$$

and:

$$\mathbf{R}=\begin{bmatrix}\cos\omega & -\sin\omega\\ \sin\omega & \cos\omega\end{bmatrix}. \tag{A9}$$

The angle ω, in the rotation matrix $\mathbf{R}$, can be written in terms of the deformation components:

$$\omega=\frac{D_{21}-D_{12}}{D_{11}+D_{22}}=\frac{\gamma(k_1-k_2)}{\ln(k_1/k_2)(k_1+k_2)} \tag{A10}$$

Thus, the length of the long and short axes of the finite-strain ellipse, the diagonal elements of matrix $\mathbf{T}$, can be given completely in terms of deformation components. The same approach could be used for a right polar decomposition.

The unified deformation matrix for plane strain, eq. (6), has been tested numerically using a computer program which gives an approximate solution by successively premultiplying small increments of pure and simple shear. As the increment size decreases, the solution converges to eq. (6). Similar tests have verified the three-dimensional strain matrix given by eq. (30) in this paper. It should also be emphasized that the analysis presented here applies only to steady state flows. However, unsteady flows can also be modeled by multiplying incremental deformation matrices with gradually changing k and γ values.

Appendix 2

Two dimensions

If $k_1 = k_2$, then:

$$D_{12} = k_1 \gamma_{xy}$$

Three dimensions

If $k_1 = k_2 \neq k_3$, then:

$$D_{12} = k_1 \gamma_{xy}$$

$$D_{23} = \gamma_{yz}\left(\frac{k_1 - k_3}{\ln(k_1/k_3)}\right)$$

$$D_{13} = \gamma_{xy}\left(\frac{k_1 - k_3}{\ln(k_1/k_3)}\right) + \frac{k_1\gamma_{xy}\gamma_{yz}}{\ln(k_1/k_3)} + \left(\frac{(k_3 - k_1)\gamma_{xy}\gamma_{yz}}{\ln^2(k_1/k_3)}\right)$$

If $k_1 \neq k_2 = k_3$, then:

$$D_{12} = \gamma_{xy}\left(\frac{k_1 - k_2}{\ln(k_1/k_2)}\right)$$

$$D_{23} = k_2 \gamma_{yz}$$

$$D_{13} = \gamma_{xz}\frac{(k_1 - k_2)}{\ln(k_1/k_2)} + \left(\frac{(k_2 - k_1)\gamma_{xy}\gamma_{yz}}{\ln^2(k_1/k_2)}\right) + \left(\frac{\gamma_{xy}\gamma_{yz}k_2}{\ln(k_1/k_2)}\right)$$

If $k_1 = k_3 \neq k_2$, then:

$$D_{12} = \gamma_{xy}\left(\frac{k_1 - k_2}{\ln(k_1/k_2)}\right)$$

$$D_{23} = \gamma_{yz}\left(\frac{k_2 - k_1}{\ln(k_2/k_1)}\right)$$

$$D_{13} = \gamma_{xz}k_1 - \frac{k_1\gamma_{xy}\gamma_{yz}}{\ln(k_2/k_1)} - \left(\frac{(k_2 - k_1)\gamma_{xy}\gamma_{yz}}{\ln(k_1/k_2)\ln(k_2/k_1)}\right)$$

If $k_1 = k_2 = k_3$, then:

$$D_{12} = k_1\gamma_{xy}, \quad D_{23} = k_1\gamma_{yz}, \quad D_{13} = k_1\gamma_{xz} + (k_1\gamma_{xy}\gamma_{yz})/2$$

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