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StrainModeler: A Mathematica™-based program for 3D analysis of finite and progressive strain

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ABSTRACT

StrainModeler is a program constructed in the Mathematica™ environment that performs 3D progressive strain calculations for lines and planes undergoing any sequence of homogeneous deformations. The main inputs to the system define the initial line or plane to be deformed and the deformation sequence to be applied, including combinations of simple shear, pure shear and volume change. For the deformation of lines, the output of the program is the change of attitude of the initial line, which can be represented by graphics or plotted in an equal-area projection. For the deformation of planes, the program has several outputs: (i) change of attitude of the initial plane; (ii) magnitudes and ratio of the semi-axes of the strain ellipse on the deformed plane; (iii) orientation of the major and minor axes of the strain ellipse on the deformed plane; (iv) orientations of the axial planes of the folds formed on the deformed plane, and (v) area change on the deformed plane. The variation of any of these parameters can be shown against a linear parameter only linked to the number of steps involved in the deformation, as a kind of "time" line, or it can be shown against the variation of a parameter of the strain ellipsoid (e. g.: major axis/minor axis ratio). A sequence of directions can be also visualized as a curve in an equal-area plot. Three applications of the program are presented. In the first, the deformation by simple shear of a plane with any orientation is analyzed. In the second, we explore the formation of recumbent folds in layers with different initial orientations for simple shear and pure shear deformations. In the third, we use StrainModeler to analyze the deformation of a set of folds located in a ductile shear zone in the Variscan Belt of NW Spain.

1. Introduction

The analysis of deformation in rocks is an essential task in structural geology. The strain of rocks is difficult to measure and its analysis must be made by approximations based on several types of homogeneous strain. Two types of approaches exist for the analysis of deformation:

a) Analyze the strain variation throughout the rock volume. In this approach, the strain at each material point within the rock must be considered. For example, this is the method used to study the state of strain in a folded layer to determine the kinematical folding mechanisms. In this case, the analysis is made by linearization of the transformation involved in the deformation. Homogeneous strain in small rock volumes is assumed in this approach. This is the method used for example by Hudleston and Holst (1984), Holst and Fossen (1987) and Bobillo-Ares et al. (2004).

b) The whole-rock strain approach. This assumes that the boundaries of a large rock volume are deformed following the rules of homogeneous strain or simple inhomogeneous strain, although inside the body the strain is usually inhomogeneous. For example, if we say that a rock body has been deformed in a homogeneous simple shear regime, we assume that the boundaries of this body are deformed according to this type of strain. If this body is layered, the layers will have undergone shortening or stretching depending on their initial orientation in relation to the deformation and on the character of the bulk deformation. The shortening or stretching of the layers can be inhomogeneous, and it can give rise to the development of folds or boudins respectively (see, for example, Ramsay, 1980). In the case of development of folds, it is assumed that the median surface of the folded layer possesses the same final orientation as the layers would have had if the strain had been homogeneous; this assumption has been assumed implicitly by several authors (e. g.: Ramsay, 1980; Carreras et al., 2005; Fossen, 2010, Fig. 15.31) and has been tested in numerical experiments by Llorens et al. (2013). In this paper, we mainly follow this approach (b).

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The types of strain histories usually considered in the analysis of the natural deformations of rocks are the following:

a) Progressive simple shear. This is an isochoric (no volume change) non-coaxial strain history with the following properties: (1) Two families of orthogonal planes maintain their position during the deformation; (2) line segments on planes of one of these families (shear planes) do not undergo changes in length or orientation during deformation; (3) the displacements of material points take place in a single direction or its opposite. Simple shear can be homogeneous or inhomogeneous. The latter is a type of strain that has been commonly considered as a whole-rock strain for the kinematic analysis of geological structures.
b) Progressive coaxial strain. This is a strain history in which the orientations of the axes of the strain ellipsoid do not change with the deformation with respect to material lines. It can be with volume change or without volume change (pure shear).

Other types of strain history used for the analysis of the geological strain result from a combination of the above types. A type of non-coaxial strain intermediate between pure and simple shear is one in which the kinematic vorticity number (Truesdell, 1953; Means et al., 1980) is lower than that of simple shear; it is named "sub-simple shear" (De Paor, 1983; Simpson and De Paor, 1993). This has been usually defined as the result of a simultaneous combination of pure shear and simple shear. Sometimes it is interesting to consider the successive superposition of coaxial deformation on simple shear or vice versa, but in these cases it is necessary to bear in mind that the order of the superposition influences the final result. Another type of homogeneous strain history described in the geological literature is the super-simple shear (De Paor, 1983), in which the internal rotation is higher than that of simple shear; this type seems rare in crustal scale deformation (Bailey et al., 2004) and is not further considered in this paper.

Simple shear, coaxial strain and their combinations have been described in detail by many authors (e.g. Truesdell and Toupin, 1960; Ramsay, 1967, 1980; Ramsay and Graham, 1970; Ramberg, 1975; Sanderson, 1982; Tikoff and Fossen, 1993). Nevertheless, several problems related to these deformations are not yet resolved. An interesting question is related to the fact that in nature it is possible to find layers in a variety of orientations in relation to the reference axes usually used to describe the types of deformation cited above. In these cases, knowledge of the state of strain and strain history in such planar surfaces is necessary to explain some geometrical features of structures such as folds, foliation, lineations and boudins.

In addition to the finite strain, knowledge of the progressive strain has great relevance to the understanding of the development of many geological structures, whose initiation and evolution is controlled by the incremental deformation. Obtaining the variation of the main parameters that characterize the deformation of any line or plane (variations in orientation, length, etc.) as a function of the parameters of the strain ellipsoid of the whole-rock strain is one of the objectives of this paper.

Several previous contributions regarding the deformation of lines and planes in a 3D deformation are noteworthy. Equations relating the rotation of planes and lines to the deformation of the rocks containing them were obtained by Flinn (1962) using the deformation ellipsoid. He also borrowed the Fresnel construction from optical mineralogy to determine the attitude and length of the principal axes of shortening and extension in any plane. Ramsay (1967, p. 154–158) presents equal-area projections contoured for longitudinal strain that facilitates an easy analysis of these concepts. Lisle (1986) analyzed the non-coaxiality that appears in the deformation of a plane which is inclined to the principal axes of the strain ellipsoid in the case of a 3D coaxial deformation.

Carreras (1975) applied the simple shear displacement function to a planar surface inclined at any angle to the shear zone to obtain the relationship between angles and shear strain. This relationship was used by him to develop graphical and numerical methods to determine shear strain from angular measurements of structural elements of shear zones. In a similar line, Skjernaa (1980) obtained equations for the reorientation of randomly oriented planes and lines during progressive homogeneous simple shear.

Ramberg (1976) obtained equations for the orientation and the length of the principal axes of the elliptical intersection between a strain ellipsoid and a plane and Ramberg and Ghosh (1977) analyzed the rotation and progressive strain of a sheet embedded in a matrix which undergoes rotational 3D strain under constant volume conditions. They obtained equations that can be used to calculate the following: (i) the position and length of the principal axes of the strain ellipsoid at any stage of the deformation; (ii) the position and length of the principal axes of the strain ellipse in any plane at any stage of the deformation; (iii) the position and length of passive markers which initially coincided with the principal axes of the strain ellipse in a plane and then rotated passively; and (iv) the shear strain parallel to a plane or sheet.

Treagus and Treagus (1981) developed methods to determine the orientation and length of the principal axes of the strain ellipse in layers oblique to the axes of the strain ellipsoid both in the case of known initial orientation and known deformed orientation. These methods were used to analyze the obliquity between the fold axes originated in the layer and the *XY* plane of the 3D deformation.

Vollmer (1988) developed a computer model to deform homogenously a quasi-planar surface with several initial perturbations, and used it to analyze the formation of sheath-nappes in the Norwegian Caledonides. To model the deformation, the surface is divided in a set of quadrilaterals, each of which being a small planar element which is homogeneously deformed. Davis and Titus (2011) give a review of computational techniques for homogeneous steady deformation and apply the matrix exponentials and logarithms method to solve two problems: a forward problem of constructing a new kinematic model of transpression and an inverse problem of finding the best homogenous steady model for a given set of field data.

At the present state of knowledge, a versatile and friendly computer tool that can be used to perform progressive strain calculations may be very useful for the structural geologist. In this paper, a 3D analysis of the strain resulting from any specified sequence of homogeneous deformation is presented, with special emphasis on combinations of simple shear, pure shear and volume change. Transformations that a given plane or line undergoes as a result of the deformation are analyzed. In order to automate the calculations and to visualize the results of both the finite strain and the progressive strain, this analysis has been used to develop a new program, named 'StrainModeler', in the MATHEMATICA™ environment. Two examples of the application of this software are presented. Firstly, it is used to shed light on the strain conditions of the formation of recumbent folds, and then it is applied to unravel the conditions of deformation in a sector of a kilometer-scale natural ductile shear zone.

2. Theoretical background

In this section we present the mathematics that constitutes the basis of StrainModeler. First of all, the method used to characterize the homogeneous deformation involved in the analysis is