Vorticity analysis in shear zones: A review of methods and applications. Comment

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Xypolias (2010) reviewed the methods developed in the last 30 years to quantify the shear strain in mylonites. The most prominent element in his essay appears to be his scepticism: "We have a fragile sense of confidence about numbers extracted from rocks using methods of vorticity analysis, which are still in a relatively immature stage of development". It was refreshing to this author to find doubt or uncertainty openly expressed. Far too many workers in science produce excellent data, and then try by all means to interpret them along theories by others, often enough even if their own data plainly show that the theory lacks realism. But dissent is usually not openly expressed. Practical researchers rarely speak up against theoreticians; hence the latter are often granted an authority which may be undeserved. Xypolias' statement above can be read as a verdict, even if perhaps he did not mean it that way.

Much in the mechanics of simple shear is at best incompletely understood. The obliquity of fabric diagrams (Bouchet et al. 1983) is often interpreted to indicate that the fabric did 'not yet reach the 'ideal position' in the foliation plane *XY* for infinite strain; but the angle of obliquity is surprisingly stable, and equivocal in case of minerals with multiple slip systems. The existing explanations for the kinematics of S-C-fabrics may be good for relatively small deformations, but how this fabric is generated, and evidently regenerated over and over again during extensive shear without producing interference structures, remains a mystery. The discovery of a line that divides σ-clasts and δ-clasts was a major achievement, but the interpretation given so far – superposition of simple and pure shear – remains unconvincing because a mylonite with 'ideal' simple shear parameters has not yet been found, and the volume loss or foliation-perpendicular flattening suggested by the current interpretation is always very substantial, and it is a guess; there is no other evidence for it.

In this discussion I do not wish to take issue with Xypolias' review itself, which is thoroughly exhaustive and very laudable. It is just that his stated scepticism does not reach deep enough. The unquestioned basement on which the various methods have developed is continuum mechanics. It is the flaws in this theory that find their direct expression in the confusion above.

In none of the many textbooks on the theory of stress and deformation in continuum mechanics I have seen – to name just a few of them: Cauchy (1827a, 1827b), Love (1952), Green and Zerna (1954), Truesdell (1954), Sneddon and Berry (1958), Truesdell and Toupin (1960), Sokolnikoff (1964), Landau and Lifschitz (1965), Eringen (1967), Malvern (1968), Gurtin (1972, 1981), Truesdell (1991), Holzapfel (2000) – has there been any mention of the fact that a solid is held together by bonds, at least not in the respective chapters on stress theory, and usually not at all. Bonds do not exist in continuum mechanics. Bonds are certainly mentioned in many engineering textbooks or in fracture mechanics, (e.g. Anderson 2005), but the authors are clearly not aware of an incompatibility which nonetheless exists, and which expresses itself in many ways, because the nature of elasticity itself is not understood. One cannot ponder a bond-breaking process if the bonds are not considered in the theory in the first place. To make this item absolutely clear: the first person I asked why bonds are not mentioned in stress theory, was the lecturer of my introductory class in 1980 in California. He did not answer, and no one since has given an answer. Thus, after 30 years in this field, it is not premature to ask if the emperor is really dressed.

Elastic deformation is by nature a change of state in the sense of the First Law of thermodynamics, it requires work to be done by a surrounding upon a system such that an elastic potential develops, the Helmholtz free energy. Plastic deformation is irreversible and calls for the Second Law. However, the current understanding of stress and elasticity is still firmly based on Cauchy's theory (1827a, 1827b) which was conceived 20 years before the discovery of the First Law of thermodynamics (Helmholtz, Joule); 30 years before the founding of modern linear algebra and tensor mathematics (Grassmann, Hesse); 40 years before vector fields were introduced, both as a mathematical concept and as a physical phenomenon (Maxwell, Faraday), without which a spatial theory cannot be constructed; 40 years before the thermodynamic groundwork was laid which is required to understand the interaction of system and surrounding (Clausius, Gibbs); and 50 years before atoms, and thus bonds, were accepted as real and existent (Boltzmann) – all of which is missing in Cauchy's theory. His theory is conservative in the sense of Newton's mechanics of discrete bodies in freespace. To explain this in very few words: a process which observes the energy conservation law of mechanics is said to be *conservative* because the sum $E_{kin} + E_{pot} = H = const$ is 'conserved', i.e. constant, where H is the entire energy of a system. In thermodynamics, H is called the internal energy U which is then a variable, hence the process is *non-conservative*, and the energy conservation law is $dU = dw + dq$. A non-conservative process may then be *reversible* ($dq/T = 0$) or *irreversible* ($dq/T > 0$). But a conservative approach cannot describe a non-conservative process, such as elastic loading, because it must cogently lead to the conclusion that a volume-neutral deformation does not cost physical work (Koenemann 2001, 2008a).

This author is aware of four different, conceptually independent approaches to deformation theory. Cauchy's is the oldest, and quaintest. The one by Landau and Lifschitz (1965) is much more modern mathematically, but also conservative in the sense just explained (Koenemann 2008a). The only approach in which a vector field is derived from a potential, and which is in that respect compatible with potential theory, thermodynamics and the existence of bonds, is the one by Helmholtz (1902). It is incomplete due to the author's sudden death in 1894, was worked out by his staff based on his lecture notes, and is entirely forgotten. However, it is the only approach with modern elements before Koenemann (2008b) which is fully thermodynamic.

The immediate consequence for the current discussion is that a theory of vorticity (Truesdell 1954) which ignores the most essential property of solids – bonds – and which is not applicable to changes of state, should no longer be used. It may help to realize that in all of Truesdell's writings known to this author – ditto for Gurtin, Eringen, Love, Sokolnikoff and many others – only one particular type of force can be found, which is Newton's $\mathbf{f} = m\mathbf{a}$. This is a very specific force because it cannot be derived, it is a single vector force that cannot form a field, it involves the inertial mass [kg], and it refers to the kinetic energy E_{kin} and to the acceleration of discrete bodies in freespace. Instead, the force $\mathbf{f} = \mathbf{e}_i dU/dx_i$ (U = some potential) was discovered by Lagrange in 1784, became important with the rise of electromagnetic physics from 1860 on, and is the dominant force definition in modern engineering. It is a field force, it is evidently derived, and the reference mass may be the thermodynamic mass which is dimensionless (the n in $PV = nRT$); but it has never been used in continuum mechanics, except for Helmholtz (1902). $\mathbf{f} = m\mathbf{a}$ cannot be a bonding force because bonds are a form of potential energy; continuum mechanics in its present state thus cannot consider bonds.

Vorticity studies are performed in the attempt to quantify shear, as opposed to strain. Perhaps it is the wrong question. Xypolias' review correctly represents the current state of discussion: it is clinically free of physical reasoning. Deformation is almost exclusively perceived as a geometrical "mapping" from the undeformed into the deformed state (Gurtin 1981). This it is not; deformation is a physical process that requires work to be done, and which is subjected to the principle of least work. Pure shear and simple shear are commonly seen as end members of some spectrum, but this they are not; they are two different displacement types that developed as a function of their respective boundary conditions, and which differ substantially in their respective energetics, both in the elastic and the plastic realm. The physical question that really matters is to ask how the boundary conditions in a continuum come about, and what the energetics of the various displacement types tell us. The partition of a simple shear into a pure shear and a rotation, which is so popular in structural geology, is known as the Helmholtz partition. How this partition could end up in a theory of deformation of solids, elastic or plastic, is hard to understand, because Helmholtz (1858) proposed it as a conceptual tool in a paper on the friction-free flow of a perfectly non-coherent gas. In Helmholtz (1902) it is not mentioned.

So what does the evidence found by e.g. Passchier and Simpson (1986) or Simpson and de Paor (1997) really tell us? They found an apparently stable direction far from the foliation plane XY, the only one which is intuitively perceived as stable. It expressed itself as a fabric divider, porphyroclasts on either side had undergone opposite rotation in their matrix. The initial studies gave angles of 60 to 80° from X, and inclined against the sense of shear. More recent studies tend to be very close to 69-70°. The dividing line was interpreted as a measure of superposition of pure and simple shear.

In the light of the new theory (Koenemann 2008b) a very different interpretation offers itself. What Passchier, Simpson and de Paor have found is evidence that there are bonds in solids. As pointed out above, bonds have not been considered in continuum mechanics, hence ideal simple shear was believed to be similar to laminar flow. But this type of flow would have to be friction-free; it is physically impossible in a solid. The new approach instead treats a solid as a bonded continuum, and elastic deformation as a change of state, hence it starts with an equation of state and the First Law. The interaction of the external force vector field which is subject to external boundary conditions, and the material properties, also expressed as a force vector field, plus the condition that system and surrounding are bonded to one another, result in a third field that combines their properties. This resulting force field is the equivalent to what used to be called stress, but it can have less than orthogonal symmetry properties. For boundary conditions of simple shear it is indeed monoclinic. The resulting force vector field is transformed one-to-one into the elastic displacement field (also a vector field) through the work equation, in the same way as ΔV can be calculated from PdV if ΔP is known, such that their geometric properties are identical. The force/displacement field for simple shear is characterized by two stable eigendirections in the *XZ*-plane. One of them, the contracting eigendirection, is predicted to be at 68,4° to the foliation plane, and inclined against the sense of shear. It happens to be the same direction as that of the maximum loading along the San Andreas fault at 69 ± 14° (Hickman and Zoback 2004), and the orientation of post-kinematic joints that open in deactivated metamorphic shear zones during uplift. Thus the fabric dividing line at 69-70° is right where it is expected to be. The contracting and extending eigendirections enclose an angle of 100°. The extending eigendirection is ca. 11° above the *XY*-plane and marked by the S-plane in S-C fabric, or by the alignment of elongated clasts in mylonites which do *not* reach the foliation plane with progressive deformation. The foliation plane *XY*, however, is not a plane of any particular significance at all, but a physical expression of the boundary conditions, a composite fabric element in the sense of Means (1984), and mechanically very close to a non-shearing direction. The details are outlined in the reference above, and in Koenemann (2011).

References

Anderson TL (2005) Fracture mechanics. Taylor & Francis, Boca Ration, 621 pp.

Bouchet L, Lister GS, Nicolas A (1983) Fabric asymmetry and shear sense in movement zones. Geologische Rundschau 72, 401-450.

Cauchy AL (1827 b) De la pression ou tension dans un corps solide. Exercices de Mathématiques 2, 42-56.

Cauchy AL (1827 c) Sur la condensation et la dilatation des corps solides. Exercices de Mathématiques 2, 60-69.

Eringen C A (1967) Mechanics of continua. J. Wiley & Sons, 502 pp.

Green AE Zerna W (1954) Theoretical elasticity. Clarendon Press, 442 pp.

Gurtin ME (1972) The linear theory of elasticity. Handbuch der Physik VIa/2, 1-296.

Gurtin ME (1981) An introduction to continuum mechanics. Academic Press, 265 pp.

Helmholtz H (1858) Über die Integrale der hydrodynamischen Gleichungen. Crelles Journal/Journal für die reine und angewandte Mathematik 55, 25-55.

Helmholtz H (1902) Dynamik continuirlich verbreiteter Massen. Vorlesungen über theoretische Physik. Vol.2. Barth, Leipzig, 247 pp.

Hickman S Zoback M (2004) Stress orientations and magnitudes in the SAFOD pilot hole. Geophysical Research Letters 31, L15S12.

Holzapfel GH (2000) Nonlinear solid mechanics. J. Wiley & Son, Chichester, UK, 455 pp

Koenemann FH (2001) Unorthodox thoughts about deformation, elasticity, and stress. Zeitschrift für Naturforschung 56a, 794-808.

Koenemann FH (2008a) On the systematics of energetic terms in continuum mechanics, and a note on Gibbs (1877). International Journal of Modern Physics B 22, 4863-4876.

Koenemann FH (2008b) An approach to deformation theory based on thermodynamic principles. International Journal of Modern Physics B 22, 2617-2673.

Koenemann FH (2011) The kinematics of simple shear. Submitted.

Landau, L.D, Lifschitz, E.M. (1965) Lehrbuch der theoretischen Physik. Vol.VII: Elastizitätstheorie. Akademie-Verlag Berlin, 223 pp.

Love AEH (1952) A treatise on the mathematical theory of elasticity. Cambridge University Press, 643pp.

Malvern LE (1969) Introduction to the mechanics of a continuous medium. Prentice-Hall, Englewood Cliffs, New Jersey.

Means, W.D. 1984. The concept of steady-state foliation. Tectonophysics 78, 179-199.

Passchier CW Simpson C (1986) Porphyroclast systems as kinematic indicators. Journal of Structural Geology 8, 831-843.

Simpson C De Paor DG (1997) Practical analysis of general shear zones using the porphyroclast hyperbolic distribution method: an example from the Scandinavian Caledonides. In: Sengupta, S. (Ed.), Evolution of Geological Structures in Micro- to Macro-scales. Chapman and Hall, London, pp.169–184.

Sneddon IN Berry DS (1958) The classical theory of elasticity. Handbuch der Physik VI, 1-126.

Sokolnikoff IS (1964) Tensor analysis. Theory and applications to geometry and mechanics of continua. Wiley & Sons, 361 pp.

Truesdell CA (1954) The Kinematics of Vorticity. Indiana University Press, Bloomington.

Truesdell CA (1991) A first course in rational continuum mechanics. Second edition, Academic Press, 391 pp.

Truesdell CA Toupin RA (1960) The classical field theories. Handbuch der Physik, Vol.III/I, 266-858, Springer Verlag.

Xypolias P. (2010) Vorticity analysis in shear zones: A review of methods and applications. Journal of Structural Geology 32, 2072-2092.