Nonlinear structures in layered, viscous rock

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Abstract

We examine the influence of the migration of chemical constituents, driven by gradients in normal stress, upon the evolution of fold geometry in anisotropic, linearly-viscous, multi-layered materials. The layering consists of an alternating sequence of high viscosity, chemically mobile rock and lower viscosity, chemically immobile rock. In a natural analogue, the high viscosity, chemically mobile layers could be quartz rich whilst the low viscosity, chemically immobile layers could be mica rich The deformation is assumed to be incompressible, with temporarily and spatially evolving volume fractions of the mobile and immobile constituents. We present a large deformation formulation for a layered, viscous material.. The particle-in-cell finite element method combines many of the advantages of traditional finite elements with the geometrical flexibility of pure particle methods. The method is particularly suitable for problems involving very large deformation without the need for re-meshing**.**

Introduction

Within the geological record there is evidence of numerous processes where creeping flow of solid materials dominates the deformation. We often only see this evidence once the region has been uplifted, eroded, and exposed, so evidence for deformation is indirect (deformed material interfaces, physically or chemically modified grain size distributions and so on). One of the most successful ways to understand these long-completed deformation processes is forward modelling from the proposed initial state following material interfaces and the temperature / pressure/ stress and chemical histories of material elements. In the following we revisit a subject which has attracted significant attention from the structural geology community over the past 25 years, namely, pressure dissolution fuelled mass transport during inhomogeneous, and in particular, buckling-type deformations.

Geological motivation

There are many examples in deformed rocks where segregation of chemical constituents has accompanied the deformation of rocks. The process was first documented in deformed rocks by Sir Charles Darwin in the first half of the nineteenth century who described mineralogically differentiated layering associated with slaty cleavage cross cutting bedding and parallel to the axial planes of folds. Examples in the literature span the complete spectrum from simple segregation of material in the spaces between boudins through transport of material from the limbs to the hinges of folds, through to segregation of contrasting mineralogies during the formation of slaty cleavage, schistosity, and, in particular, crenulation cleavage. We are concerned with such metamorphic differentiation processes accompanying the folding of multi-layered materials and the influence these processes have upon the evolution of fold geometry.

 We examine the influence of the migration of chemical constituents upon the evolution of fold geometry. Chemical migration is driven by gradients in the normal stress across the layered

material and there is a feedback relation between the segregation of chemical species and the rheology of the multi-layered material undergoing folding. In particular, since the most common forms of metamorphic differentiation occur in highly anisotropic rocks, we concentrate on the folding of muti-layered, anisotropic, viscous materials. The folding is driven by the contrast in shear viscosities measured parallel to the layers rather than the more common situation in the literature where the folding is driven by contrasts in the "normal" viscosities between the layers. Migration of chemical constituents is driven by the gradients in normal stress that arise as the layers change orientation during folding. The changes in rheology that arise because of chemical migration have a feedback on the folding process so that changes in fold geometry arise during the segregation process. We explore the growth of non-periodic fold trains. Here we introduce viscosity softening during deformation, resulting in the development of localized shear zones which control the position of fold hinged in subsequent deformation. This process leads to the development of non-periodic fold trains.

Numerical method

The problems of interest all involve very large deformations. Simulation algorithms must therefore be able to deal with very large strains associated with the folding and compositional evolution, while faithfully tracking material history and interfaces. Versatility and robustness are usually associated with the various formulations of the Finite Element Method (FEM). The need to track material history strongly suggests a Lagrangian formulation, which provides a reference frame, locked with the material itself. Unfortunately, large deformations are quite difficult to handle within the FEM because mesh distortion and remeshing are required to maintain optimal element configurations. The Particle-In-Cell (PIC) scheme is a hybrid numerical method which falls somewhere between the Finite Element Method (FEM) and a purely Lagrangian particle method such as the Discrete Element Method (DEM). The PIC scheme attempts to combine the versatility of the continuum FEM with the geometrical flexibility of DEM. In PIC we use Lagrangian particles together with an Eulerian mesh as shown schematically in Figure 1. The mesh is used to solve nodal point velocities and pressures using almost exactly the same formulation as the standard FEM, however, the mesh is not required to track material deformation , thus avoiding the problem of mesh distortion. For problems where displacements are needed, the particles are used to integrate velocities and carry configuration information. Where internal orientations need to be tracked, as in this case, they are represented on the particles and integrated into a stiffness matrix for each element. Moresi et al., (2000 [1]), give
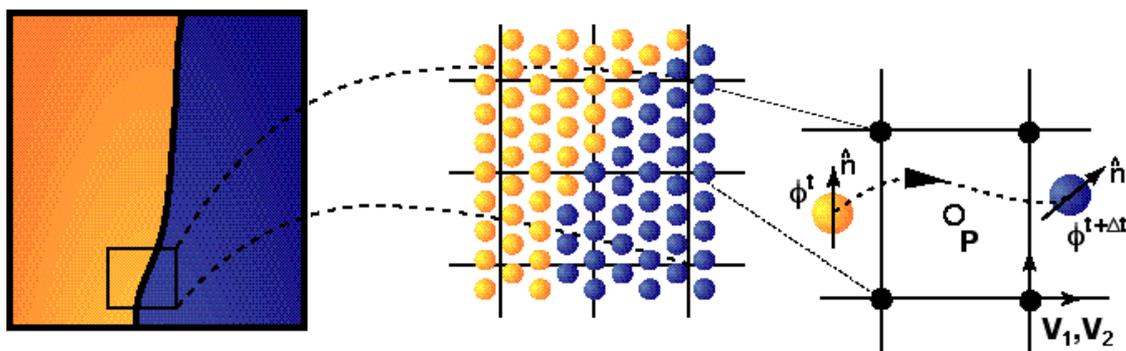

Figure 1. A schematic of the particle-in-cell approach for modeling interfaces and material orientation variations during the evolution of the solution geometry. The mesh is fixed while the particles flux through.

Mathematical formulation

From a mechanical point of view, the salient feature of layered materials is that there exists a distinguished orientation given by the normal vector field $n_i(x_k,t)$ of the layer planes, where (x_1, x_2, x_3) are Cartesian coordinates, and t is the time. We assume linear viscous behaviour and designate with h the normal viscosity and h_S the shear viscosity in the layer planes normal to n_i. The orientation of the normal vector, or director as it is sometimes called in the literature on oriented materials, changes with deformation. Using a standard result of continuum mechanics, the evolution of the director of the layers is described by

$$\dot{n}_i = -v_{k,i}\, n_k + (v_{j,k}\, n_j n_k)n_i \tag{1}$$

where the superscribed dot designates the material time derivative, v_i are the components of the velocity vector, and the comma followed by an index denotes partial differentiation with respect to the indicated Cartesian coordinate.

The most convenient way to derive the stress-stretching relation is to write down the strain rate potential with tensor components referred to Cartesian coordinates chosen parallel to the material symmetry axes. The gradient of the potential with respect the stretching components referred to the global system is obtained as:

$$s_{ij} = 2hD'_{ij} - 2\Delta h(n_i n_m d_{lj} + n_j n_m d_{il} - 2n_i n_j n_l n_m)D'_{lm} - p d_{ij} \tag{2}$$

Here D_{ij} is the symmetric part of the velocity gradient (the stretching tensor),

$$D'_{ij} = D_{ij} - \frac{1}{3}\, D_{kk}\, d_{ij} \tag{3}$$

is the deviator of D_{ij}, d_{ij} is the Cartesian metric or unit tensor, p is the pressure or average stress, taken positive in compression as is usual in geology and $Dh = h - h_S$. The matrix representation of (1) and (2) is given in the Appendix for easy reference. We complete the constitutive description with an assumption regarding the rate of volume change. The usual assumption is of course $D_{kk} = 0$ which is entirely appropriate for most problems involving large deformations. Elastic or shear strain controlled dilatancy relations as used in soil mechanics are not relevant at the time and deformation scales envisaged here. However there is ample evidence for significant mass transport in folded rocks where the transport can not be readily explained on the basis of conventional constitutive concepts (e.g. Hobbs et al 1976[2]). A widely accepted explanation for such changes in local composition is that matter (usually quartz) is dissolved along layer interfaces with relatively large normal stress and precipitated along interfaces with relatively low normal stress. Dissolution and precipitation provides a positive feedback to the folding process itself.

We propose that the net volume change is zero however we admit local changes in composition and mass transport. Before we put this into equations we have to specify the rheological nature of the layering. We consider an alternating sequence of high viscosity and low viscosity materials which are chemically mobile (dissolvable) and immobile respectively. The volume fractions are f^m and f^{imm}, $f^m + f^{imm} = 1$ and the viscosities are given as (e.g. Biot, 1964[3]; Johnson and Fletcher, 1994[4]):

$$h = f^m h^m + (1 - f^m)h^{imm} \text{ and } h_S = \frac{h^{imm} h^m}{f^n h^{imm} + (1 - f^m)h^m} \tag{5}$$

The total velocity in (1) and (2) is the weighted average of the velocities of the two constituents, whereby the volume fractions are the weighting functions. Assuming that the total volume and hence the total density is constant yields:

$$D_{kk} = v_i,_i = (\boldsymbol{f}^m v_i^m),_i + ((1-\boldsymbol{f}^m)v_i^{imm}),_i = 0 \tag{6}$$

However, within the confines of (6), the volume fractions may vary spatially and temporarily. We complement (6) by a mass conservation equation for the mobile constituent. We assume that the material time rate of the volume fraction $\boldsymbol{f}^m$ is controlled by the in-layer gradient of the normal stress traction. This expresses the observation that the layer interfaces serve as conduits for mass transport, fuelled by pressure dissolution at the layer interfaces. We have:

$$\acute{\boldsymbol{f}}^m = -(\frac{\boldsymbol{l}k}{Et}(\boldsymbol{s}_n,_k - \boldsymbol{s}_n,_l\, n_l n_k)),_k \quad \text{where} \quad \boldsymbol{s}_n = -n_i n_j \boldsymbol{s}_{ij} \tag{7}$$

where k is the in-layer permeability, dimension *(length)²*, E is the Young's modulus, $\boldsymbol{t}$ is the time scale at which the mobile phase dissolves in the interstitial fluid under stress and $\boldsymbol{l}$ is a matching parameter. If $\boldsymbol{n}^T=(0,0,1)$ and the parameters k and $\boldsymbol{h}^m$ are constant then (7) reduces to

$$\dot{\boldsymbol{f}}^m = -\frac{k}{\boldsymbol{h}^m}(\boldsymbol{s}_n,_{11} + \boldsymbol{s}_n,_{22}) \quad \text{where} \quad \boldsymbol{s}_n = -\boldsymbol{s}_{33} \tag{8}$$

Mass transport does not take place if the in-layer Laplacian of the normal stress vanishes; the phases are in equilibrium with their own solutions. If gradients exist, the mobile phase is transported down the normal stress gradient. In folding scenarios this means transport away from the limbs-towards the hinges. In (2) and (8) we have tacitly assumed that $\boldsymbol{s}_{ij}$ is equal to the effective stress. In the following examples we will always assume that the excess pore pressure is equal to zero at the time scale of the processes of interest. Inclusion of pore fluid flow would merely complicate the algebra.

Numerical simulations

We present an example of a simulation of folding of a layer of anisotropic viscous material sandwiched between two isotropic layers. The ratio of normal viscosity between embedded layer and the background is a factor of 20. The shear viscosity of the central layer is one fortieth of the normal viscosity. The orientation of the internal layering is approximately parallel to the macroscopic layering of the system with some small perturbations ($\boldsymbol{dq} \le \boldsymbol{p}/50$) have been introduced at a very fine scale. The assumption is that the sample represents a pristine geological formation with no prior deformation history recorded in the layering so that any folding response is not biased to an imposed lengthscale. The boundary conditions in this case are slippery, undeforming boundaries on the vertical sides and the base, and a free surface at the top of the layers (not shown). No density variations are assumed in this case.

In a simulation with purely isotropic materials, the viscosity contrast between the embedded layer and the background is insufficient to observe any folding for a simulation with 50% shortening.

In Figure 2, the influence of anisotropy in the embedded layer can clearly be seen. Fine scale perturbations to the layer orientation develop very early in the shortening, and soon amplify into disturbances in the layer interfaces. The amplification disrupts the periodicity at an early stage so that the deformation of the interfaces occurs at a number of different wavelengths. After approximately 30% shortening, a dominant wavelength is apparent in the folding, but smaller scale structure inhereted from the early stages of folding is still present and continues to grow. This results in an extremely complex deformation pattern at the termination of the experiment.
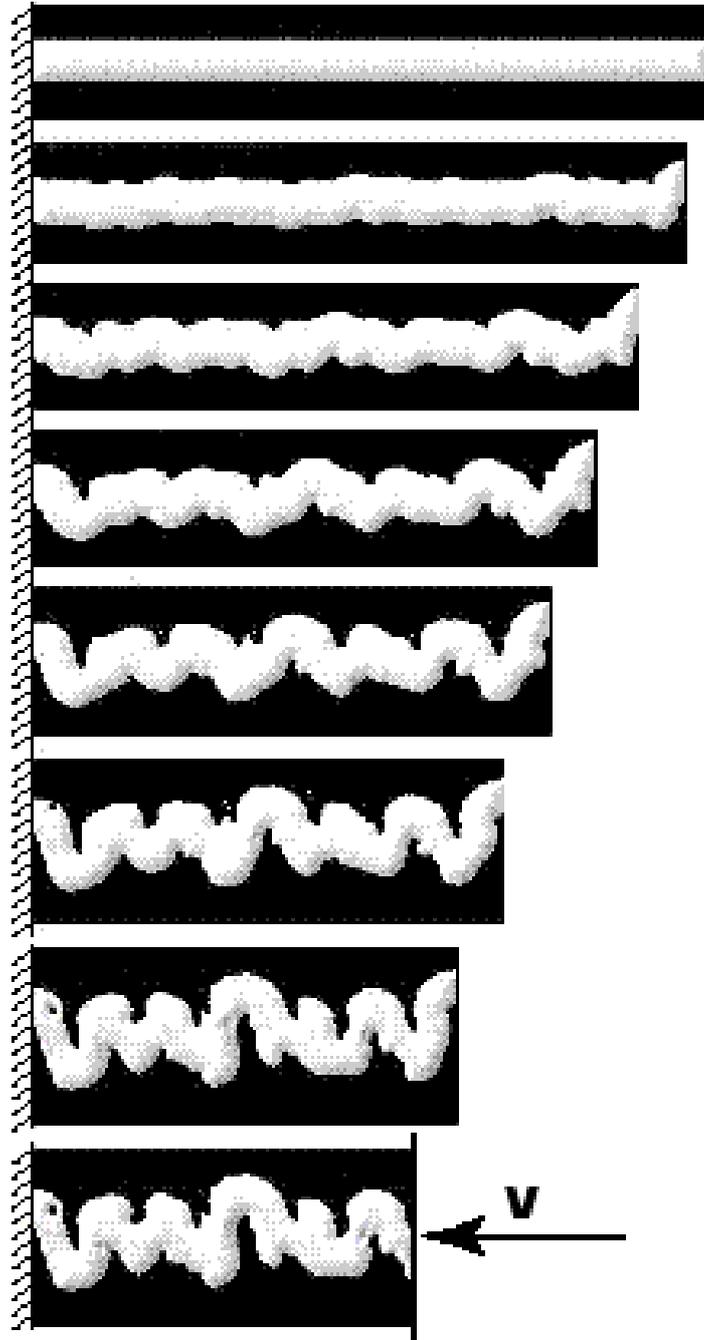

Figure 2. An embedded layer of anistropic viscous material embedded in an isotropic, low viscosity background undergoes 50% shortening.

These behaviours can be understood with the help of a linear instability analysis which predicts the modes of instability in the small deformation limit. The competition between these modes is played out as the deformations become large, however, which is the natural domain of computational simulation.

Summary

We have presented a simple formulation for the inclusion of chemical migration into deforming layered systems. The combination of the basic model with a large deformation, particle-in-cell finite element method allows the simulation of a diverse range of crustal deformation problems. Our demonstration examples include a realistic treatment of folding which includes the mechanical influence fine-scale laminations and the dissolution/precipitation of soluble materials during deformation. A linear instability analysis gives a good insight into the expected modes of deformation at the onset of instability. Further simulations which include the effects of chemical transport will also be presented.

References

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