NUMERICAL APPROACHES TO LARGE-SCALE GEOLOGICAL MODELING

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Summary
Geological deformation problems which arise when studying thermal mechanical evolution of the Earth's crust and lithosphere have much in common with the dynamics of complex fluids. Rocks deform as visco-elastic-plastic materials and typically we are interested in studying very large strains, post failiure deformation, and tracking structural evolution. Particle-in-cell codes have proven very successful in this field. They cope well in tracking large- strain deformation, interface tracking and following material history, while at the same time, efficient and robust parallel solvers can be constructed more easily on a structured background grid.

INTRODUCTION

On a geological timescale, and at the pressures and temperatures found in the deep crust and mantle, rocks deform as visco-elastic fluids with a tendency to undergo shear-localization at high stresses. Many open questions in geology relate to the development of crustal structure in response to far-field plate stresses and convective motions in the deep lithosphere and mantle. Numerical challenges resulting when modelling these processes arise from the emergence of complicated structure, from the fine-scale structure and strong rheological contrasts associated with localisation, and the history dependence of the constitutive behaviour which needs to be followed through very large strains. A fluid-dynamics formulation of the geological deformation problem begins with the Stokes' equation describing the balance of viscous stresses and pressure gradients with bouyancy forces. To first order, the deformation can be considered incompressible.

$$\tau_{ij,j} - p_{,i} = f_i \tag{1}$$

where $\boldsymbol{\tau}$ is the deviatoric stress tensor, p is pressure, and $\boldsymbol{f}$ a buoyancy force term. For an isotropic viscous material, the deviatoric stress and the strain-rate, $\boldsymbol{D}$ are related through the viscosity η as

$$\tau_{ij} = 2\eta D_{ij} \tag{2}$$

Viscoelastic-plastic deformation can be included as a modified viscosity and a contribution to the right hand side:

$$\eta \leftarrow \eta^{\text{eff}}; \;\; \eta^{\text{eff}} = \frac{\eta^{\text{vp}}\mu\Delta t_e}{\eta^{\text{vp}} + \mu\Delta t_e} \tag{3}$$

$$f \leftarrow f + f^{\text{el}}; \;\; f^{\text{el}} = -\frac{\eta_{\text{eff}}}{\mu\Delta t^e}\tau^t_{ij,j} \tag{4}$$

where μ is the elastic shear modulus, η^{vp} is the viscosity, here including viscoplasticity, and Δt^e is an time increment which resolves elastic relaxation. Full details are given in Moresi et al. [2003] including the extension to more complicated plastic flow rules. For our purposes, it is sufficient to note that η^{vp} develops strong spatial gradients due to localisation and is dependent on the material history, and f^{el} is a tensorial stress history term evaluated with the moving fluid.

METHODS

A particle-in-cell Finite Element Method is used to study these problems. Particles (points which track material position and a local orientation) flux through the finite element mesh during fluid flow. The trajectories of the particles is computed from the solution of the Stokes equation on the mesh points. The constitutive behaviour and stress-history contributions to the right hand side are computed by using the (effectively) random particle positions within each element to construct a quadrature rule. The approach is related to the Material Point Method [Sulsky et al., 1994, Sulsky and Brackbill, 1991]. The Stokes equation is discretised on a highly regular mesh of quadrilateral / hexahedral elements. Preserving regularity allows us to implement an efficient, parallel (geometrical) multigrid solver using the PETSc system [Balay et al., 2004]to provide smoothing / solver parameters which can be tuned at runtime. The incompressibility constraint is enforced by a combination of Augmented Lagrangian methods [Glowinski and Tallec, 1989, Fortin et al., 1983] and a Schur-complement reduction [May and Moresi, 2008].

EXAMPLE: SHEAR BAND FORMATION

A viscous material with a Drucker-Prager yield criterion is sheared with constant velocity boundary conditions. There is a 20% reduction in the material cohesion over a plastic strain of 0.1. An random perturbation in the initial damage is introduced to seed localisation at the center of the domain. Figure (1A) shows the resulting shear band orientation as a

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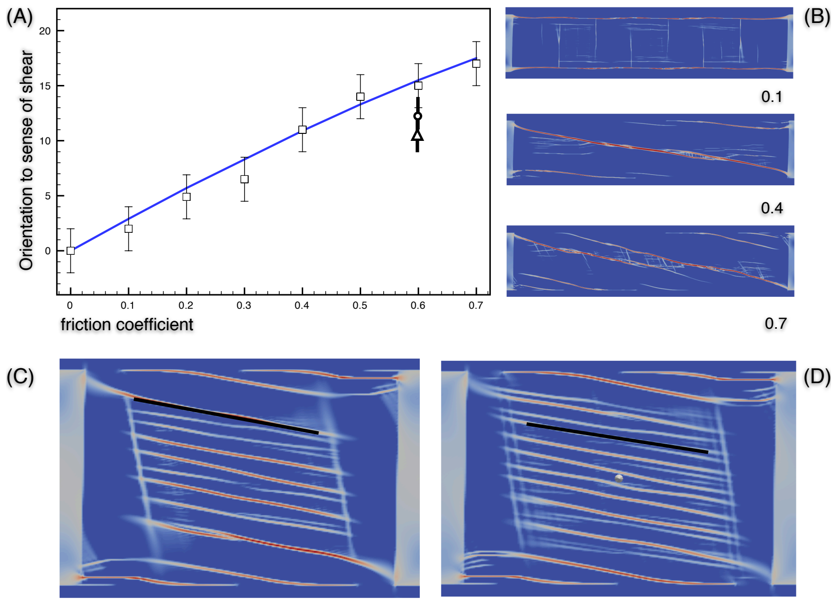

Figure 1. Shear band orientation with simple-shear boundary conditions. (A) The orientation of shear bands as a function of the friction coefficient. 2D results are indicated by open squares; the 3D results are indicated by the circle (C) and triangle (D). (B) Two dimensional results showing the strain-rate pattern after a total shear (at the boundaries) of 2%. (C and D) planform of 3D experiments with a layer thickness of 10% of the layer width. The sample material is bounded by a low viscosity layer above and below in case (C) and by a low viscosity and intermediate viscosity material in case (D). There is no effect of gravity in any models.

function of the friction coefficient. Shear bands form close to the Coulomb angle in the 2D case. In the 3D cases, we find that the shear bands can be much shallower than this (and the shear bands orientations vary within the sheared layer). Here the only effects we have considered are: the finite thickness of the sample layer and the strength of the material in which the layer is embedded.

CONCLUSIONS

Our numerical approach allows us to study geological deformation problems from initially small deformation to very large strains and to follow interface evolution and localisation without significant loss of efficiency. We have developed fast, robust solvers which exploit the regularity / unchanging topology of the grid for parallel decomposition and simplicity of implementation.

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