Simulating fluid injection in geological media with complex rheologies

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Abstract. Stimulation of geothermal systems by injection of water into wells at high pressures to create fractures and increase permeability of rocks is a widely used technique. Therefore, increasing our understanding about how such actions influence the local state of stress of the reservoir and how fractures propagate through it is necessary to efficiently develop extraction projects and, hopefully, to avoid undesired side effects. Advances in numerical modelling of hydraulic fracturing are thus required. To that end, we improved the modelling and solving capabilities of the software LaMEM by adding plasticity, poroelasticity and Darcy flow making this code capable of simulate dilatant materials, accounting by the angle of dilatation, and reproduce shear/tensile failures due to local pore pressure increase. This improvement offers us an efficient computational massively-parallel code to model fluid injection and crack propagation in poro-visco-elasto-plastic rocks. Here we give examples of such model.

1. Introduction

In order to simulate geological processes such as lithospheric deformation it was developed LaMEM (Lithospheric and Mantle Evolution Model), a scalable 3D parallel code that employs a staggered finite difference discretization combined with a marker and cell approach. This software solves, in an efficient way, the (incompressible) Stokes equations in rheologies involving rocks that have nonlinear visco-elasto-plastic material properties. In particular, this code is able to model the formation of localized shear bands during planar deformation in agreement with theoretical and experimental results [1].

However, it is well know that liquid pressure in porous rocks plays an important role in processes such enhanced geothermal systems as it influences the state of stress of the reservoir (e.g. [2], [3]) and, thus, must be considered when modelling deformation and failure. Here, we take advantage of LaMEM and follow previous ideas [4], [5] to implement Darcy flow and couple it with the Stokes equations in order to account for liquid pressure in porous rocks. In addition, as such processes develop at relatively low temperatures, when the mechanical behavior is almost elasto-plastic, we improved plasticity by adding the dilation angle of rocks and by implementing tensile failure, one of the possible failure modes due to local pore-fluid overpressuring and/or extensional forces.

In section 2, we describe the physical model used for this purpose and its numerical implementation. Next, in order to validate the code, we will show some results looking for
shear/tensile bands formation and how the dilation angle influences in the angle of localization (3.1) and for the reproduction of the main failure modes resulted from fluid injection (3.2).

2. Physical and numerical approach

We consider a continuous media under the effect of gravity \( g \) composed by poro-visco-elasto-plastic rocks with properties density \( \rho \), shear modulus \( G \), bulk modulus \( K \) and viscosity \( \mu \). To describe the main factors acting in the medium we use Cauchy stresses \( \sigma_{ij} \), pressure \( P \), deviatoric stresses \( \tau_{ij} \) and temperature \( T \) and, to describe deformation, velocities \( v_i \), strain rates \( \dot{e}_{ij} \) and its poro-elastic, viscous and plastic descomposition

\[
\dot{e}_{ij} = \dot{e}^{pe}_{ij} + \dot{e}^{v}_{ij} + \dot{e}^{p}_{ij}
\]

Here, \( i \) and \( j \) refers to coordinate indexes \( (x,y,z) \). We assume that pores are connected and filled, in a measure given by the permeability \( k \) and the specific storage \( S_p \) properties, by a liquid of density \( \rho_l \) exerting pressure \( P_l \) on rocks. We define, then, the effective pressure of the system as

\[
P_{eff} = P - P_l
\]

In addition, we assume the existence of a limit for rock stresses, the scope of which produces plastic failure and is defined by cohesion \( C \), friction angle \( \phi \) and tensile strength \( \sigma_T \). The combined yield criteria for shear ([6]) and tensile failure ([7]) that we use is given by (figure 1)

\[
\tau_{yield} = \min \left( P_{eff} \sin \phi + C \cos \phi, P_{eff} + \sigma_T \right)
\]

and the plastic behavior is defined by the plastic flow potential ([8], [9])

\[
Q = \tau_{II} - P_{eff} \sin \psi
\]

being \( \psi \) the dilation angle indicating the relation between the plastic volumetric strain rate and the rate of plastic distortion ([8])

\[
\sin \psi = \frac{\dot{\epsilon}^{p}_{NN} + \dot{\epsilon}^{p}_{YY} + \dot{\epsilon}^{p}_{ZZ}}{2 \dot{\epsilon}^{p}_{II}}
\]

and considering \( \psi = 90^\circ \) for tensile failure. The expressions \( \tau_{II} \) and \( \dot{\epsilon}_{II}^{p} \) denote the second invariant of the deviatoric stress and the plastic strain rate, respectively. If yield is reached, the plastic strain rates are given by

\[
\dot{\epsilon}_{ij}^{p} = \chi \frac{\partial Q}{\partial \sigma_{ij}} = \dot{\epsilon}_{II}^{p} \left( \tau_{II} + \frac{2}{3} \sin(\psi) \delta_{ij} \right)
\]

being \( \chi \) multipliers satisfying the yield condition

\[
\tau_{II} = \tau_{yield}.
\]

We solve the mass, momentum and energy conservation equations for the solid skeleton affected by the liquid pressure,

\[
\frac{\partial T}{\partial t} - \frac{1}{K} \frac{\partial P}{\partial t} + 2 \sin(\psi) \dot{\epsilon}_{II}^{p} = \frac{\partial v_i}{\partial x_i}
\]
The yield criteria for the second invariant of the deviatoric stress considered for plastic failure in equation (3) is plotted as black line. $P'$ indicates the effective pressure corresponding to the intersection between the line $t: P_{\text{eff}} + \sigma_T$, that forms an angle of $45^\circ$ with respect to the horizontal axis, and the line $s: P_{\text{eff}} \sin \phi + C \cos \phi$, with an angle of $\arctan(\sin \phi)$. Its analytical value is $P' = (\sigma_T - C \cos \phi)/(\sin \phi - 1)$. On the other hand, the set of all the semicircles with center $P_{\text{eff}}$ and radius $\tau_{\text{yield}}(P_{\text{eff}})$, plotted in red for tensile and in blue for shear, defines the yield criteria for shear stress and is given by a combination between the semicircle corresponding to $P'$ (in red) and the line $r: P_{\text{eff}} \tan \phi + C$ with angle $\phi$. Such envelop is plotted in green colour. The effective pressure corresponding to the intersection point ($P_I$) can be calculated as $P_I = (-b + \sqrt{b^2 - 4ac})/(2a)$ where $a = \tan^2 \phi + 1$, $b = 2C \tan \phi - 2P'$ and $c = C^2 - (P' + \sigma_T)^2 + P'^2$.

and the mass conservation equation combined with the Darcy's law for liquids

$$\frac{\partial \tau_{ij}}{\partial x_i} - \frac{\partial (P + \alpha P_i)}{\partial x_i} + \rho g_i = 0$$

(9)

$$\rho C_p \frac{dT}{Dt} = \frac{\partial}{\partial x_i} \left[ \frac{1}{2} \frac{\partial T}{\partial x_i} \right] + H$$

(10)

**Figure 1.** The yield criteria for the second invariant of the deviatoric stress considered for plastic failure in equation (3) is plotted as black line. $P'$ indicates the effective pressure corresponding to the intersection between the line $t: P_{\text{eff}} + \sigma_T$, that forms an angle of $45^\circ$ with respect to the horizontal axis, and the line $s: P_{\text{eff}} \sin \phi + C \cos \phi$, with an angle of $\arctan(\sin \phi)$. Its analytical value is $P' = (\sigma_T - C \cos \phi)/(\sin \phi - 1)$. On the other hand, the set of all the semicircles with center $P_{\text{eff}}$ and radius $\tau_{\text{yield}}(P_{\text{eff}})$, plotted in red for tensile and in blue for shear, defines the yield criteria for shear stress and is given by a combination between the semicircle corresponding to $P'$ (in red) and the line $r: P_{\text{eff}} \tan \phi + C$ with angle $\phi$. Such envelop is plotted in green colour. The effective pressure corresponding to the intersection point ($P_I$) can be calculated as $P_I = (-b + \sqrt{b^2 - 4ac})/(2a)$ where $a = \tan^2 \phi + 1$, $b = 2C \tan \phi - 2P'$ and $c = C^2 - (P' + \sigma_T)^2 + P'^2$.

and the mass conservation equation combined with the Darcy's law for liquids

$$\frac{\partial}{\partial x_i} \left( \frac{k}{\mu} \frac{\partial P_i}{\partial x_i} \right) + \left( \rho_1 g \right) \right) + H_i = \frac{D P_i}{D t}$$

(11)

considering the poro-visco-elastic-plastic constitutive relation to describe deviatoric changes

$$\dot{\varepsilon}'_{ij} = \frac{1}{2G} \frac{D \tau_{ij}}{D t} + \frac{\tau_{ij}}{\tau_T} + \frac{\tau_{ij}}{\tau_H} \frac{D \tau_{ij}}{D t}$$

(12)

Here, $x_i (i = 1,2,3)$ are the spatial coordinates, $D/Dt$ is the material time derivative, $\dot{D}/Dt$ is the Jaumann derivative, $\alpha_T$ is the thermal expansion coefficient, $\alpha$ is the Biot-Willis constant and $H$ and $H_2$ are possible head or liquid sources, respectively. We refer readers to [1] in order to get the details for the definition of elastic and viscous part of deviatoric strain rates.
Equations (8) to (11) have been discretized in space by using staggered grid finite differences method. To achieve scalability on massively parallel machines have been used the distributed arrays (DMDA) and iterative solvers (KSP, SNES) from the PETSc library ([10]). A Marker And Cell method has been employed to track material properties which are advected in an Eulerian kinematical framework. We refer readers to [1] for the details of the LaMEM implementation.

3. Results

3.1. Elasto-Plastic Benchmark - Angle of shear bands

Among others, shear band formation of elastoplastic soil samples, where friction and cohesion control planar deformation, was theoretically studied in [11]. The author reviewed what were then the current theories about preferred orientation of shear bands (e.g. [12], [13], [14]) and concludes, by means analytical and experimental data, that shear bands for a material with friction angle \( \phi \) and dilation angle \( \psi \) are oriented, with respect to the direction of the minor principal stress, at an angle that varies, depending of the particle size and elastic unloading, between the Roscoe angle \( 45^\circ + \psi/2 \) [13] and the Coulomb angle \( 45^\circ + \phi/2 \) [12]. This range includes the Arthur or intermediate angle \( 45^\circ + (\phi + \psi)/4 \) proposed in [14].

Numerical experiments done by [15], [16], [17], [18], [5] have similar results for non associated incompressible flow (\( \psi = 0 \)) while [19] demonstrated that the Coulomb angle is the preferred orientation of shear bands if an associated plastic flow rule is considered, where the plastic potential function and the yield function coincide since in such case \( \phi = \psi \). Here we test the influence of the implemented dilation angle on the preferred orientation of shear bands by performing uniaxial compressional/extensional simulations in a model setup consisting in an elasto-plastic domain with 40 km length, 0.625 km width and 10 km height. A viscous heterogeneity 0.8 km long, 0.625 km wide and 0.4 km high is introduced at the bottom so that the shear bands start there. We impose free surface at the top and zero normal velocity and free slip at the bottom. Properties of the materials, numerical parameters and sketch of the model setup are given in tables 1 and 4 and figure 2, respectively.

| Variable | Parameters | Value | Units |
|----------|------------|-------|-------|
| \( \rho \) | Density | 2700 | kg m\(^{-3}\) |
| \( G \) | Shear module | \( 5 \times 10^{10} \) | Pa |
| \( v \) | Poison’s ratio | 0.30 | |
| \( C \) | Cohesion | 40 | MPa |
| \( \phi \) | Friction angle | 30 | \(^\circ\) |
| \( \psi \) | Dilation angle | \([0,10,30]\) | \(^\circ\) |
| \( \sigma_T \) | Tensile strength | 20 | MPa |
| \( \mu \) | Viscosity of weak inclusion | \( 10^{14} \) | MPa s |
First, we run simulations considering a fixed friction angle $\phi = 30^\circ$ and varying dilation angles to $\psi = 0^\circ$, $\psi = 10^\circ$ and $\psi = 30^\circ$ and subject the medium to lateral compression by imposing a constant background strain rate of $10^{-25} \text{s}^{-1}$ until bands clearly localize. In all simulations we measure the angle between the shear band and the horizontal axis, therefore, as in the case of compression the minimum principal stress is vertical, the theoretical Roscoe, Coulomb and Arthur angles with respect to the horizontal axis are $45^\circ - \psi/2$, $45^\circ - \phi/2$ and $45^\circ - (\phi + \psi)/4$, respectively. Figure 3 shows the second invariant of the strain rate tensor for the different dilation angles and table 2 gives a summary of the expected and resulted shear angles for each case. We observe that dilation decreases the angle of shear bands significantly, moving it towards the Roscoe and the Arthur angles.
Figure 3. Simulations of shear bands localization due for a lateral uniaxial compression of a medium described in table 2 and figure 1 using numerical parameters indicated in table 4. We plot in first, second and third rows the second invariant of the strain rate tensor resulting of considering dilation angles $\psi = 0^\circ$, $\psi = 10^\circ$ and $\psi = 30^\circ$, respectively, and a fixed friction angle $\phi = 30^\circ$. We measured the angles of shear bands by looking for the maximum strain rate on the horizontal line at 0.6 km and 2.6 km from the centre of the domain. Comparison with theoretical results are showed in table 2.

Next, we subject the same model to extension by means of a constant background strain rate of $10^{-15}$ s$^{-1}$ for the case $\phi = 30^\circ$, $\psi = 10^\circ$. In order to compare the initiation of bands close to the surface, for the compressional and extensional case, we plot in figure 4 the second invariant of the strain rate tensor and Mohr-Coulomb circles for some specific points resulting of the simulations. We can appreciate that for the compressional case (first row) only shear bands form whereas tensile fractures appear in the extensional one (second row). If extension is maintained for longer shear localization occurs forming an angle of $55^\circ$ with respect to the horizontal axis.

In all cases, results are as expected from the physical formulation and the position in the yield criteria, therefore, we conclude that the code is able to consider in a correct way the dilation angle.
Figure 4. Second invariant of the strain rate tensor, yield criteria and pressure-deviatoric stress state resulting of simulating lateral uniaxial compression/extension of a medium described in table 1 and figure 2 using numerical parameters indicated in table 4. For all simulations we consider friction angle $\phi = 30^\circ$ and dilation angle $\psi = 10^\circ$. First row shows the initiation of shear bands for the case of compression and pressure-stress state at the central point of the squares superposed in the domain. Squares and semicircles on the graphic are related each other by colour and show the locally measured stress state together with the yield stress envelop. Second and third rows show the results for the case of extension at two different time stages of the simulation. Tensile fractures appear in these cases and shear localization is produced as in the case of compression. We measured the angle and compared results in the same way as in figure 3.

Table 2. Theoretical and calculated angles for shear bands.

|                | Friction | Dilation | Roscoe | Arthur | Coulomb | Simulation |
|----------------|----------|----------|--------|--------|---------|------------|
| Compression    | $30^\circ$ | $0^\circ$ | $45^\circ$ | $37.5^\circ$ | $30^\circ$ | $42^\circ$ |
| Extension      | $30^\circ$ | $30^\circ$ | $30^\circ$ | $30^\circ$ | $30^\circ$ | $31^\circ$ |

3.2. Poro-elasto-plastic benchmark - Failure patterns

Some studies (e.g. [4]) show that a local increase in pore pressure affects the mode in which poro-elasto-plastic rocks fail. In the next test, we therefore consider a 4000 m length, 62.5 m width, 1000 m height poro-elasto-plastic domain where a 50 m low permeability boundary layer is imposed at the bottom and lateral boundaries. We perform simulations subjecting the model to uniaxial compression or extension at the time that liquid is injected at the centre of the bottom boundary in order to decrease effective pressure in this area. The properties of the materials, numerical parameters and sketch of the model setup are given in table 3, 4 and figure 5, respectively. Figure 6 shows the resulting failure modes for an extension of $10^{-14}s^{-1}$, a compression of $10^{-10}s^{-1}$ and an extension of $10^{-12}s^{-1}$ constant background strain rates. We can observe that first and second cases fail in shear mode whereas the last one produces a vertical tensile failure.

Table 3. Material parameters employed in the poro-elasto-plastic benchmark.

| Variable | Parameters   | Value  | Units  |
|----------|--------------|--------|--------|
| $\rho$   | Density      | 3100   | Kg m$^{-3}$ |
| $\rho_l$ | Liquid density | 1000   | Kg m$^{-3}$ |
| $G$      | Shear module | $2.4 \times 10^2$ | MPa |
| $\nu$    | Poisson’s ratio | 0.30   |        |
| $C$      | Cohesion     | 30     | MPa    |
| $\phi$   | Friction angle | 35     | $(^\circ)$ |
| $\psi$   | Dilation angle | 10     | $(^\circ)$ |
| $\sigma_T$ | Tensile strength | 10     | MPa    |
| $k$      | Permeability | $10^{-15}$ | m$^2$  |
| Parameter                  | Value                                |
|----------------------------|--------------------------------------|
| Permeability bottom/lateral boundaries | $10^{-17}$ m$^2$                     |
| $S_s$ Specific storage       | $10^{-4}$ MPa$^{-1}$                  |
| $H_m$ Source magnitude       | $[4\times10^{-3}, 4\times10^{-2}, 4\times10^{-2}]$ m$^3$s$^{-1}$ |

**Figure 5.** Model setup used for the poro-elasto-plastic benchmark.

**Figure 6.** Simulations of failure patterns due for a lateral uniaxial compression/extension plus fluid injection in a medium described in table 3 and figure 5 using numerical parameters indicated in table 4. Plots show second invariant of the strain rate tensor and arrows denote the velocity field.
Table 4. Numerical resolution and PETSc options employed in the simulations. For all of them we use Eisenstat Walker algorithm for SNES solver and FGMRES for KSP.

| Parameter                        | For figure 3 | For figure 4 | For figure 6 |
|----------------------------------|--------------|--------------|--------------|
| Numerical resolution            | 200x2x50     | 400x2x100    | 150x2x50     |
| Absolute convergence tolerance  | -snes_atol   | 1x10^{-7}    | 1x10^{-15}   | 1x10^{-7}    |
| Relative convergence tolerance  | -snes_rtol   | 1x10^{-4}    | 1x10^{-15}   | 1x10^{-4}    |
| Maximum number of iterations    | -snes_max_it | 100          | 500          | 100          |
| Absolute convergence tolerance  | -js_ksp_atol | 1x10^{-14}   | 1x10^{-14}   | 1x10^{-14}   |
| Relative convergence tolerance  | -js_ksp_rtol | 1x10^{-10}   | 1x10^{-10}   | 1x10^{-10}   |
| Maximum number of iterations    | -ksp_max_it  | 100          | 500          | 100          |

4. Conclusions
We presented a new 3D massively parallel software capable to simulate deformation and failure in poro-visco-elasto-plastic rocks. We demonstrated that the code accounts for the dilation angle in agreement with theoretical results and is able to model the main patterns of failure due to localized liquid overpressure. Further benchmark we are doing by modelling more complex setups and by applying the code to reproduce real geothermal projects and results will be presented in the future.

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