Investigation of hydro-mechanical processes in fluid-saturated fractured rock based on numerical model generation

N Pollmann¹,², J Gallas¹, M Ch Brandenburg³, L Witte¹ and T Backers¹

¹ Engineering Geology and Rock Mass Mechanics, Institute of Geology, Mineralogy and Geophysics, Ruhr-Universität Bochum, DE-44801 Bochum, Germany
² since Feb. 2021: DMT GmbH & Co. KG, Am TÜV 1, DE-45307 Essen, Germany
³ Nonlinear Algebra Group, Max Planck Institute for Mathematics in the Sciences, DE-04103 Leipzig, Germany

E-mail: nele.pollmann@rub.de

Abstract. To realistically simulate fluid flow in fractured rock mass, a scheme to represent the discrete fracture networks (DFN) in the numerical model is of utmost importance. In this paper we discuss a workflow to implement a field-measurement based DFN into an FEM code (COMSOL Multiphysics) by means of a MATLAB routine. This workflow is involved in the ZoKrateS project which aims at showing the feasibility to enhanced fractured carbonate Rock Mass by proppant placement for geothermal application.

The model generation is based on analytical geometry including the equations for dip, azimuth and spacing of lines. The spacing between the discontinuities and the characteristic fracture length and aperture as well as orientation serve as input parameters for the model. It is possible to generate periodic models to be able to include periodic boundary conditions in simulations. In 2D the fractures are modeled as poroelastic ellipses in a poroelastic square-matrix. We investigate hydro-mechanically triggered fluid transport in stationary fractures that are mechanically and hydraulically active.

An extension to 3D fracture networks requires an algorithm based on analytical geometry including the equations for azimuth, dip and spacing of planes. To decrease the numerical costs of the 3D simulation a diffuse interface approach is strived for, including a modified model generation.

With the numerical model generator (NUMOG) a workflow is developed which allows numerical investigations of (thermo-) hydro-mechanically triggered fluid transport in a geothermal reservoir.

1. Introduction

The ability to forecast thermo-hydro-mechanical properties of subsurface rock mass is of importance for geothermal reservoir application, but is also relevant for other geotechnical subsurface applications, such as carbon capture storage, hydrogen storage, hydrocarbon reservoir exploitation or deposition of nuclear waste. A suitable estimation of processes in a fractured geothermal reservoir requires adequate modeling of the fracture network. The development of a workflow that transfers field measurements into a numerical model is recently discussed, e.g. in [1, 2] where scanline data are used to create two-dimensional discrete fracture networks (DFN).
The modeling of the fluid transport in these fractures embedded in rock and the related effect of thermo-hydro-mechanical coupling is important e.g. to predict stimulation induced seismic events [3]. A considerable amount of literature has been published on the aim at modeling hydraulic stimulation using computational mechanics. These studies include Biot’s theory of poroelasticity [4] resulting in patchy saturation or double porosity models [5, 6, 7], where both, the rock and the fractures are modeled as poroelastic regions with different material properties. A large and growing body of literature has investigated sharp or diffuse interface formulation for fractured rock. Here the fractures are modeled as interfaces embedded in a poroelastic rock [8, 9, 10, 11, 12, 13]. With these approaches it is possible to derive a time-dependent stress-strain response of the models. The models are chosen small enough to reduce the numerical costs but large enough to be representative for the reservoir behavior. The results of the simulation can be used to derive effective hydro-mechanical properties of the reservoir e.g. via Computational Homogenization [14, 15].

The aim of the underlying study is to combine the methods of computational modeling and a workaround for the transfer of field measurements into DFN in a numerical model generator (NUMOG). We aspire to create a toolbox that directly combines the input data from field with different available computational modeling approaches to create a numerical application. This application can be simulated in COMSOL Multiphysics with only a short preprocess concerning the meshing. The focus of the underlying paper is on the mathematical implementation of the NUMOG.

2. Methodology
In this section we present the main approach of thermo-poroelasticity for diffusion in fractured rock. The interested reader can find more details on the general modeling of poroelastic media e.g. in [16, 17]. We investigate hydro-mechanically triggered fluid transport in stationary fractures that are mechanically and hydraulically active.

2.1. Model formulation for fractured rock
Here, the classical theory of (thermo-) poroelasticity is applied to define a rock containing domains with varying geometrical and physical parameters, considered as fractures. Both (the fractures and the rock) are modeled as poroelastic material saturated with water. It can be shown that this approach is feasible for fractures with an aspect ratio of aperture versus length of $10^{-3}$ [18]. The general formulation of thermo-poroelasticity is based on Biot’s quasi-static equations of linear consolidation neglecting body forces [19]. This set of partial differential equations uses the deformation of the solid skeleton $\mathbf{u}$, the fluid pore pressure $p$ and the temperature $\vartheta$ and reads

\begin{equation}
-\mathbf{\sigma}(\varepsilon[\mathbf{u}], p, \vartheta) \cdot \nabla = 0 \tag{1a}
\end{equation}

\begin{equation}
\dot{\Phi}(\varepsilon[\mathbf{u}], p, \vartheta) + \mathbf{w}_M(\nabla p) \cdot \nabla = 0 \tag{1b}
\end{equation}

\begin{equation}
\dot{\vartheta} + \mathbf{w}_h(\nabla \vartheta) \cdot \nabla = 0 \tag{1c}
\end{equation}

Here, (1a) is the equilibrium equation, (1b) the fluid mass balance of the pore fluid and (1c) the energy balance. The constitutive equations are derived for the case of isotropy as

\begin{equation}
\mathbf{\sigma}(\varepsilon[\mathbf{u}], p, \vartheta) := E : \varepsilon[\mathbf{u}] - \alpha p \mathbf{I} - K \alpha_s (\vartheta - \vartheta_0) \mathbf{I}, \tag{2a}
\end{equation}

\begin{equation}
\mathbf{w}_M(\nabla p) := -K \nabla p = -\frac{k}{\eta} \mathbf{I} \nabla p, \tag{2b}
\end{equation}

\begin{equation}
\mathbf{w}_h(\nabla \vartheta) := -\kappa \nabla \vartheta = -\frac{\Psi}{\rho c_v} \nabla \vartheta, \tag{2c}
\end{equation}

\]
where the total stress includes the fourth order elasticity tensor \( E \) of the undamaged material depending on the shear modulus \( \mu \) and the bulk modulus \( K \) of the dry solid skeleton. Biot’s coefficient is given as \( \alpha = 1 - K/K_s \), including the bulk modulus of the solid grains \( K_s \). Darcy’s law (2b) applies the permeability \( k \) and the fluid viscosity \( \eta \). Fourier’s law (2c) relates the thermal diffusivity \( \kappa \) to the effective conductivity \( \Psi \) and the heat capacity \( \rho c_v \). The storage function is given according to [19, 20] as

\[
\Phi(\varepsilon[u], p, \vartheta) = \frac{\dot{p}}{M} + \alpha \text{tr}(\dot{\varepsilon}) - \chi \alpha_s \dot{\vartheta} - \phi(\alpha_f - \alpha_s) \dot{\vartheta}
\]  

where \( \alpha_{s,f} \) is the volumetric thermal expansion coefficient for the solid and fluid, \( \phi \) is the porosity, the intrinsic compression compliance of the pore fluid is \( \beta = \frac{\phi}{K_f} + \frac{\alpha - \phi}{K_s} \), and the strain tensor is given as \( \varepsilon[u] := (u \otimes \nabla)_{\text{sym}} \).

These equations are the fundamentals for the computational modeling upon which the alluded approaches of sharp and diffuse interface modeling are based.

3. Generation of fracture models

We develop a scheme to transfer the data of the geological setup into a numerical model. The goal is to implement a field-measurement based DFN into an FEM code (COMSOL Multiphysics) by means of a MATLAB routine.

3.1. Two-dimensional setup

Field measurements provide information on fracture sets described by a number of attributes, such as orientation (2D: dip \( \phi \), 3D: azimuth or strike \( \phi \) and \( \theta \)), length \( l \), aperture \( \tau \) and spacing \( s \) between the fractures of one set. Thus, the NUMOG is based on these input parameters. Due to the direct link to COMSOL it is possible to perform straightforward different numerical simulations of field-measurement based DFN. The process in Matlab is based on analytical geometry including the equations for dip and distance (spacing) of points/lines. We generate points with certain spacing and attributes. These points are used as center points for the ellipses/ellipsoids that constitute the fractures in the numerical model. The first point is randomly located (\( M_i \) in Fig. 1a) in the chosen square. Then the point \( M_i' \) is derived on a parallel line with given spacing \( s \) by applying

\[
M_i' = M_i + s \cdot R^T, \quad \text{with} \quad R = \begin{pmatrix} \sin(\phi) \\ \cos(\phi) \end{pmatrix},
\]

where \( \phi \) is the measured mean dip of the fracture set. Second, visualized in Fig. 1 b), a line segment is generated on the derived parallel line which is bounded by the edges of the unit square with intersections \( v_1 \) and \( v_2 \). The length of this line can be derived by

\[
f = \sqrt{(x_{v_1} - x_{v_2})^2 + (y_{v_1} - y_{v_2})^2}.
\]

With this information we can now generate a new point \( M_{i+1} \) that is arbitrarily placed on this line (see Fig.1c)). The generated point \( M_{i+1} \) is taken as the next source point to compute an additional point with the certain spacing and dip within the square. If \( f \) is smaller than a chosen minimal value the process changes direction as shown in Fig.1d). Here, \( f \) is too small thus the point \( M_{i+2} \) is generated on a parallel line with given spacing \( s \) in the other direction, taking the first point \( M_i \) as source point. Again, we can now generate a new point \( M_{i+2} \) that is arbitrarily placed on the line parallel to the source line.

Based on the poroelastic approach, explained in detail in Sec.2, we generate ellipses with a high aspect-ratio in a square matrix. The input parameters are used to stochastically generate ellipses.
Figure 1. Generation process with input parameter $\phi$, $s$ and edge length of the square. The point $M_i$ and the input dip are taken to create a point located arbitrarily on a parallel line. If the length of the derived line segment $f$ is too small, the next point is generated in the other direction of the source point.

within a certain range, depending on the min, max or mean values of the field measurements. The points derived in the first step serve as center points of the ellipses that constitute the fractures of one set in the rock. Different sets are generated equivalently and added to the matrix. The other parameters of these ellipses, such as the length of the semi-axes and the dip are arbitrarily chosen between the input parameter range. This allows a slight, natural orientation and description of the fractures as shown exemplarily in Fig.2. The periodic character of the NUMOG can be suppressed what may however lead to shorter fractures than measured in the outcrop scan line due to ellipses cut by the edges of the unit square. The periodicity of the fracture system can be visualized by copying the model and string it together at its edges as shown in Fig.3 for three geological sets.

3.2. Three-dimensional setup

The three-dimensional part of the NUMOG is based on the same approach as in two dimensions, see Fig.4 and 5. Here, additional parameters are required such as the azimuth and the third axis. In virtue of the numerical costs in the three-dimensional modeling, the NUMOG has two options to generate the fractures. In the first option the fractures are modeled as ellipsoids, to be able to apply a classical poroelastic approach as explained in Sec.2 (set $10^{-3}$). The second option does not model ellipsoids but parametric surfaces, which can subsequently be simulated by applying a diffuse interface approach.

The NUMOG generates various sets with input parameters measured in the field. As in 2D the first point $M_1$ is randomly located within the cubic matrix of a given edge length and accordingly periodically distributed. The further points are generated arbitrarily on planes parallel to the source plane with point $M_1$ and given azimuth $\phi$ and $\theta$ by automatic selection of appropriate
midpoints inside the cubic matrix satisfying

$$M_{i+1} \in \ker(R) + M_i + s \cdot R^T,$$

with

$$R = \begin{bmatrix} \sin(\theta) \cos(\phi) \\ \sin(\theta) \sin(\phi) \\ \cos(\theta) \end{bmatrix},$$

where $\ker$ is the kernel of the matrix $R$.

For the FE model, the points are taken as center points of ellipsoids (or parametric surfaces) that constitute the fractures in the rock. The other parameters of these ellipsoids are arbitrarily chosen between the input parameter range. This allows a slight, natural orientation and description of the fractures as is done in 2D. Analogue to 2D, the periodic character of the NUMOG can be suppressed, as is done in Fig.4 and 5 for simplification.

4. Application example

We present exemplary fracture system data gained from a field study using the scanline method [21]. The data was recorded in quarries in the southern Franconian Alb about 30 km south of Nuremberg, Germany. Outcrops consisting of Upper Jurassic stratified carbonates with marl interlayers were analyzed with respect to their fracture system. A distinct system of three main spatial orientations was identified and grouped into sets. Two of these sets are semi-vertical with one striking E-W and the other striking N-S, shown in hemispherical view in Fig. 6. The third set represents the close to horizontal lying bedding which is neglected in the model. First results of the measured fracture attributes were used as input for the model, including spatial orientation, spacing, length and aperture values. These data are processed by the NUMOG to create a nonperiodical fracture model with three-dimensional fractures (ellipsoids) shown in Fig.
7. In Fig. 8 and Fig. 9 we show a part of the study area and the related numerical model. Here, some fracture sets are coloured to visualize the structure. Due to the wide range of fracture lengths within one set, the spacing of the sets was determined with respect to fracture length classes A, B, C (see Tab. 1). Thus it was possible to generate a greater convergence of the numerical model and the field measurement. The edge length of the model is chosen \( l = 5 \) m, which is comparable to the proportions of the measured outcrops.

**Figure 4.** Generation of parallel planes with spacing \( s \approx 3.3 \) m. Here, \( \mathbf{M}_1 \) is the center point of the source ellipse and \( \mathbf{M}_{2,3} \) are the center points of the new ellipses with length of approx. 6.5 m.

**Figure 5.** Generation of two geological sets. Here the fractures are modeled as 3-dimensional ellipsoids.

**Figure 6.** Orientation of two main sets of fractures in Schmidt net projection. Field measurement versus numerical model.

**Figure 7.** Orientation of the two main sets of fractures in the numerical model.
Table 1. Geological sets including all input parameters based on scanline data. The ranges with min and max value are given within the square brackets.

| set | class  | spacing s [m] | length s [m] | aperture τ [m] | strike [°] | dip [°]  |
|-----|--------|---------------|--------------|----------------|------------|----------|
| 1   | A      | [1.05, 1.15]  | [0.3, 1]     | [0.006, 0.02]  | [277.5, 278.5] | [87.5, 88.5] |
|     | B      | [2.45, 2.55]  | [1.0, 1.5]   | [0.020, 0.03]  | [277.5, 278.5] | [87.5, 88.5] |
|     | C      | [3.55, 3.65]  | [2.5, 5]     | [0.050, 0.10]  | [277.5, 278.5] | [87.5, 88.5] |
| 2   | A      | [1.25, 1.35]  | [0.3, 1]     | [0.006, 0.02]  | [8, 9]    | [85.5, 86.5] |
|     | B      | [2.15, 2.25]  | [1.0, 1.5]   | [0.020, 0.03]  | [8, 9]    | [85.5, 86.5] |
|     | C      | [2.55, 2.65]  | [2.5, 5]     | [0.050, 0.10]  | [8, 9]    | [85.5, 86.5] |

Figure 8. Scanline at study area: Southern Franconian Alb circa 30 km south of Nuremberg, Germany. Outcrops consisting of upper Jurassic stratified carbonates with marl inter-layering.

Figure 9. Part of the study area and numerical model. Fracture surfaces colored by set. The stratum is neglected in the numerical model.

5. Conclusions and outlook
The aim of the investigation was to generate DFN models based on geological measurement with a MATLAB Routine. We presented the mathematical framework and the basic equations to generate the case of two- and three-dimensional ellipsoidal fractures in a square or cubic matrix. An application example was presented for a visual comparison between the numerically generated model and the field measurement. In this study area we identified two main sets which were further subdivided in length classes to be implemented in the NUMOG. We showed that the mathematical framework is able to generate DFNs that are representative and that display the recorded data. These field-based DFN models are the base for the numerical simulation with classical thermo-poroelastic equations stated in Sec. 2. The equations are already included in the MATLAB Routine of the NUMOG, as well as the variables for defining the poroelastic properties, the preparation for the meshing, different boundary conditions and the setup for the study in COMSOL Multiphysics. Thus, the NUMOG generates a COMSOL file, including all necessary model parameters, based on the input data that is processed by Matlab. For the sake of brevity this was not explained in detail in this paper and remains a promising area for further work on the numerical simulation. The implementation of the further alluded computational methods in the NUMOG is in progress.
All in all we announced a mathematical framework for the generation of numerical DFN including the basic equations with a direct link to the FE software COMSOL Multiphysics depending on outcrop scanline data.

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