DETERMINATION OF THE PLASTIC STRENGTH OF CARBONATES FROM MICROTOMOGRAPHY AND THE UPSCALING USING PERCOLATION THEORY

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Keywords: plastic strength, carbonate, microtomography, percolation theory, upscaling

Abstract. In this paper we establish a workflow for upscaling of rock properties from microtomography using percolation theory and focus on the plastic strength of rocks. The novel aspects of this study are: (1) determining the size of the mechanical representative volume element by using upper/lower bound computations based on thermodynamics; (2) using FEM to simulate the rock yielding at microscale, two cases of different pressures of linear Drucker-Prager plasticity of rocks are simulated, then the cohesion and the angle of internal friction of the rock are obtained; (3) detecting critical exponents of mechanical parameters from a series of derivative models that created by a shrinking/expanding algorithm, and then deriving scaling laws. We use a microtomographic data set of a carbonate sample to test the procedures. The preliminary results are promising.
INTRODUCTION

Understanding the physics of porous rocks is a challenge for the industry with economical interest in hydrocarbon resources, geothermal energy and mining. Microtomography enables the detection of internal structure of rocks on micro- to nano-scales and opens a new way to quantify the relationship between the microstructure and their mechanical and transport properties. Numerical computations of microtomographic data have shown good agreement with experimental data for fluid flow and elastic properties [1, 2]. However, the extension of the methodology to plastic properties is still a poorly understood area. Owing to the finite size of microtomographic images, the higher the resolution, the smaller is the length scale of the sample that is contained in a certain number of pixels or voxels. This leads to the immediate challenge to detect the internal structure of rocks across micro to nano scales and at the same time connect the images to the macro-scale essential for describing the petroleum, geothermal or mining reservoir.

In this paper we establish a workflow for upscaling of rock properties from microtomography using percolation theory and apply this to the plastic strength of rocks. A microtomographic dataset of a carbonate sample is used to test the workflow.

1.1 Workflow

Our work starts from the gray scale images of microtomography and involves three main components based on the binary data obtained after image segmentation (see Figure 1). The binary data have only two phases -- pores and solid, being represented by 0 and 1, respectively. Three main components in the workflow are:

1) geometrical analyses (left column) – it conducts quantitative analysis including stochastic analysis of the geometry of the model. General parameters, such as porosity, connectivity, specific surface area, and the fractal dimension are obtained. Stochastic analysis outputs probabilities of porosity, percolation, and anisotropy of different sizes [3]. The size of representative volume element (RVE) can be determined when the probabilities converge with the increase of the size analyzed. Permeability of rock is directly related to the geometrical characteristics, thus the geometrical RVE is suitable for computing permeability.

2) mechanical analyses (middle column) – in this component, we determine the size of mechanical RVE by detecting the mechanical responses of maximum and minimum (upper and lower bounds) entropy productions of models of different sizes [4, 5]. Then the plastic response of the microstructural model is analyzed over the mechanical RVE. We will explain this component in detail in the next sub-section.

3) extracting critical exponents of key parameters of rock property – here we use a shrinking/expanding algorithm [6] to create a series of derivative models with different porosity. From percolation theory, some parameters (including permeability, elastic modulus, yield stress, and more) change exponentially when the porosity is approaching the percolation threshold [7 - 10]. The exponential index describing this tendency is the critical exponent of the parameter.

With any two critical exponents and/or the fractal dimension, scaling laws are defined. Scaling laws, the percolation threshold, and some other parameters such as crossover length (refer to [6]) are constraints used for upscaling properties from micro-scale to large scale. The workflow is suitable for properties of fluid flow and mechanics. In our previous study [3, 6], the determination of geometrical RVE and the upscaling of permeability are verified using a sandstone sample. In this paper we focus on deriving mechanical material parameters with the workflow.
1.2 Focus of this paper

The first focus of this paper is the determination of the mechanical RVE. We use the thermodynamic upper and lower bound principles postulated in Regenauer-Lieb et al. [4, 5] to quantify whether our computations of the mechanical response of models with different sizes have converged such that they can deliver homogenized values. Upper bound corresponds to a constant displacement boundary condition; lower bound corresponds to a constant force boundary condition. Theoretically, upper and lower bounds give different responses for models of small size; the difference diminishes as the model size increases (see Figure 2). The size of mechanical RVE is determined from the converging solutions. To demonstrate the workflow, we calculate mechanical properties such as elasticity and plasticity and we assume for simplicity that the elastic response can be used to derive the size of the mechanical RVE.

Figure 2: Thermodynamic homogenization of upper and lower bounds of microstructures (from [4]).
The second focus is the computation of plastic strength of microstructures. We use linear Drucker-Prager plasticity and the finite element method to simulate the rock yielding for a mechanical RVE. In order to conduct cohesion and the angle of friction of rock samples, two cases of different pressures are simulated. Using the relationship of

$$\sigma_y = \sigma_n \tan \varphi + c,$$  (1)

where $\sigma_y$ and $\sigma_n$ are yield stress and normal stress computed from Drucker-Prager plasticity, $c$ and $\varphi$ are cohesion and the angle of internal friction of the rock, with two groups of $\sigma_y$ and $\sigma_n$ results of the model, $c$ and $\varphi$ are deduced.

The third focus of this paper is to extract critical exponent of yield stress. Shrinking/expanding algorithms [6] are used to create a series of derivative models with different volume fractions. The percolation threshold $p_c$, which is the lowest volume fraction when there exists an unbroken structure connecting at least two opposite outside boundaries for a finite volume, can be detected from these derivative models. Then the derivative models close to the percolation threshold are used to simulate the deformation and yielding. With a series of results of yield stress of models, it is possible to fit the critical exponent of yield stress $T_y$ in the form of

$$\sigma_y = (p - p_c)^{T_y},$$  (2)

when the volume fraction $p$ is approaching the percolation threshold. $T_y$ is a scale-independent parameter describing the change of yield stress for all scales.

2 IMPLEMENTATIONS AND RESULTS

We use a publicly available microtomographic dataset of a carbonate sample to test the workflow. The dataset was downloaded from http://www3.imperial.ac.uk/earthscienceandengineering/research/perm/porescalemodelling. It is a segmented binary RAW format dataset of the size of 400-cube voxels. The resolution of a voxel is 2.9 µm [11]. The porosity is 23.3% and the 3D rendering of the structure can be seen in Figure 3.

2.1 Mechanical RVE

Sixteen cubic volumes of sizes from 40-cube to 400-cube are analyzed (voxel as unit in the following unless specified). Each volume that is smaller than 400-cube is arbitrarily selected from the 400-cube model but it is ensured the porosity is $23 \pm 0.5\%$.

Two kinds of meshes are used for these volumes for finite element computing. Hexahedral elements are used for small volumes (side-length $L < 100$), which are easy to create and the computing time is acceptable. Tetrahedral elements are used for large volumes ($L > 100$). This
entails extra procedures and manual work to create but can dramatically reduce the computing time. For the volume of \( L = 100 \), we used both to compare the difference caused by mesh. While creating tetrahedral element meshes, we considered the balance of keeping the precision and the fineness of the mesh and reducing the computing time.

For all these computing models, we used the same boundary constraints. That is, surfaces (refer to Figure 4a) \( x = x_0, y = y_0, \) and \( z = z_0 \) are displacement constrained in normal direction; surfaces \( x = x_m \) and \( y = y_m \) are free. Constant normal convergent displacement and compressive pressure loads are applied on the surface \( z = zm \) for each computing model, corresponding to upper and lower bounds, respectively. The displacement value on the boundary is 0.01% of the \( L \). The pressure value on the boundary is 0.05 GPa. Displacement boundary conditions and loads are chosen such that no large deformation or plastic deformation occurs. The input elastic parameters of solid are: Young’s modulus \( E = 50 \) GPa, Poisson’s ratio \( v = 0.2 \). Abaqus® is selected to perform all the finite element computations. Two meshes of the computing models are shown in Figure 4b and 4c.

![Figure 4](image)

Figure 4: (a) A computing volume and its coordinate system; (b) mesh of the 100-cube volume, hexahedral elements; (c) mesh of the 100-cube volume, tetrahedral elements.

Young’s modulus and Poisson’s ratio of the computed model are calculated from the output of Abaqus® by using the equation

\[
\varepsilon_{ij} = \frac{1}{E} \left[ (1 + v)\sigma_{ij} - v\sigma_{kk}\delta_{ij} \right],
\]

where each stress component \( \sigma_{ij} \) is the average value of all elements in the model, strain components \( \varepsilon_{ij} \), however, are average displacements on surfaces divided by the side-length of the model. It gives us different results of \( E \) and \( v \) when use displacements on different surfaces \( x = x_m, y = y_m \) and \( z = zm \). Corresponding to the boundary conditions we used, elastic modulus calculated from the displacement on the surface of \( z = zm \) is reasonable and reliable. In contrast, Poisson’s ratio is more reasonable from the surfaces of \( x = x_m \) and \( y = y_m \). We use the averaged Poisson’s ratio of the results from these two surfaces.

Figure 5 shows the tendency of the elastic modulus and Poisson’s ratio of the upper and lower bounds of different volume sizes. Although they are not ideal as indicated in Figure 2, lower bounds are lower than the upper bounds from a certain minimum volume onwards, except 2 values of \( L \) for Poisson’s ratio in Figure 5. These two exceptions do not refute the upper and lower bound principles according to the physical definition of Poisson’s ratio. Convergence can be seen for the volume size larger than 320. Thus, the mechanical RVE is determined as 320-cube voxels for this carbonate sample. The convergent values are \( E \cong 32 \) GPa and \( v \cong 0.26 \). Thus the elastic modulus of this porous structure is 64% of the pure solid; and the Poisson’s ratio has increased more than 20%.
2.2 Plastic strength

Simulations of plastic response are based on the mechanical RVE derived from elastic analysis – i.e. 320-cube voxel volume. Two more parameters are necessary for Drucker-Prager plasticity as input: 1) the angle of internal friction of the solid matrix, which is specified as 40° in this study; 2) cohesion, which is specified as 30 MPa. We only considered elastic perfectly plastic behaviour in our computations.

A displacement boundary condition is used on the surface at \( z = z_m \). The magnitude of displacement is fixed to 1.6 units and it allows 0.5% total strain in the \( z \) direction. As mentioned in Section 2, two cases of different pressure are analyzed to detect cohesion and the angle of internal friction of the microstructure. Case 1 uses normal constraint on surfaces \( x_0, y_0 \) and \( z_0 \); Case 2 uses a uniaxial strain condition in which all surfaces except the loading surface are normally constrained.

Finite element computations deliver the deformation, strain and stress of nodes and/or elements under the applied boundary conditions, increment by increment. For each increment of output, we calculate the average values over all elements of the model for components of stress, total strain, and plastic strain. Figure 6 shows the averaged stress-strain relationships represented by the minimum principal strain and the minimum stress for Case 1 and Case 2. Case 1 demonstrates a typical elastic perfectly plastic behaviour with the yield stress of 23 MPa. Case 2 illustrates a plastic hardening feature and no obvious yield point can be identified. In this case, the concept of offset yield point can be used, which is generally set at 0.1% or 0.2% of the strain, arbitrarily. This means that if the strain is larger than 0.1%, the model is considered as yield and the corresponding stress can be defined as yield stress.
In the post-processing we determine the angle of friction and cohesion using equation (1). We use von Mises stress and pressure of the direct output of Abaqus® at the yield point as $\sigma_y$ and $\sigma_n$. The yield point of Case 1 is identified as shown in Figure 6 the plateau; the yield point of Case 2 can be arbitrarily selected at the strain of 0.1% or 0.2%. We tried both approaches and found that they lead to similar cohesion and friction angle. In fact, even if the von Mises stress and pressure at the strain of 0.5% are used for Case 2, the results are almost the same. More information can be seen in Figure 7. For Case 1, the relationship between von Mises stress and pressure is linear before yielding occurs; both von Mises stress and pressure are constant after yielding. For Case 2, von Mises stress and pressure show a nonlinear relationship at the beginning of the deformation, and then show a linear feature. More importantly, the linear trend is connected to the point after yielding of Case 1. The linear trend implies that any two points after yielding of Case 1 and Case 2 will give us the same result of cohesion and the angle of friction. A fitted line is shown in Figure 7. The slope and the intercept are 0.2565 and 20.2, respectively. Thus the cohesion is 20.2 MPa and the angle of friction is 14.4°. Compared with the input solid parameters, the porous structure causes the reduction of the cohesion to two-thirds, and significantly decreases the angle of friction to one-third.

$$S_{\text{mises}} = 0.2565p + 20.192$$

![Figure 7: Relationship of Mises stress and pressure, and the fitting of cohesion and friction angle from points after yielding of two cases.](image)

### 2.3 Critical exponent of yield strength

In the study of elastic and plastic percolation, the connectivity of the solid phase is considered. Thus, a series of derivative models are created by shrinking the solid structure. As the volume fraction of solid $p$ is decreasing while shrinking, at some stage the connection is broken and the percolation threshold can be determined [6]. Figure 8 shows the change of the volume fraction of solid with the shrinking steps, and some images of the structure after shrinking are shown. The original model has 76.7% solid volume fraction and obviously is percolating in all three directions. After 20 shrinking steps, the structure with volume fraction less than 7% is not percolating in three directions anymore; after 24 shrinking steps, the structure is not percolating in any direction. Thus, the model of 23 shrinking steps being percolating only in one direction is defined as critical model; its volume fraction of 4.47% is recognized as the percolation threshold of the solid of this sample.

As we can see from Figure 8, there are floating blocks in the models. These floating blocks must be removed, as they do not contribute to the strength of the model but cause numerical singular problems or rigid movement in computations. After removing the floating blocks, the volume fraction is 3.3% for the critical model. Thus the percolation threshold in fact is 3.3%.
Derivative models that are above and close to the percolation threshold (No. 23) will be used to simulate the plastic response for computing the yield stress. Among these models, Nos. 20 to 22 are not percolating in all 3 directions. In this situation, the boundary constraints and loads may be hard to define because there is no solid phase on one or more outside surfaces of the 320-cube volume. No. 18 and No. 19 are percolating in 3 directions but the links in these models are too weak. The meshing procedure breaks the very weak links while accurate fine stepped surfaces are replaced by smoothed coarse triangular surfaces. Thus we analyzed derivative models of Nos. 13 to 17. The differences of volume fractions to the percolation threshold \(|p - p_c|\) (all after removing floating blocks) are in the range of 6.32% to 15.19%.

We used the boundary conditions of normal displacement being zero on surfaces \(x = x_0, y = y_0, z = z_0\), and normal displacement being 1.6 on surfaces \(x = x_m, y = y_m,\) and \(z = z_m\). The displacement loading allows 0.5% strain in each direction. Stress-strain curves under these boundary conditions are shown in Figure 9 and three analyzed derivative models are inserted. We see that as the distance from the percolation threshold increases, the value of the yield point increases. Samples with higher solids volume fraction also exhibit a distinct failure point followed by weakening behavior whereas the samples close to percolation maintain deformation at almost constant stress after the yield point.
Figure 10 shows the yield stress versus the difference of volume fraction and the percolation threshold $|p - p_c|$ in log-log plot. The fitting line gives a power of 1.33. This is the critical exponent of yield stress $T_p$ based on the analyses of derivative models of the carbonate sample. The value is much less than 2.5 obtained by Benguigui et al. [9] and even less than 1.7 obtained by Sieradzki and Li [8]. Sahimi [10] thought that Sieradzki and Li’s low value is presumably due to the fact that in their experiments samples with $|p - p_c|$ = 0.1~0.23 were not in the critical region close to $p_c$. In our numerical experiments, $|p - p_c|$ of models are in the range of 0.06 to 0.15, is similar to that of Benguigui et al.

![Figure 10: Yield stress $\sigma_y$ versus $|p - p_c|$ in a log-log plot and the fitted relationship.](image)

A distinguish feature of our models is that our models are strongly heterogeneous, compared with those of previous laboratory models. Results of finite element computing show us that significant stress concentrations are around some weak links. These weak links are rare and irregularly distributed, especially for the models very close to $p_c$. These few points of stress concentration determine the eventual yield of the volume. We speculate this might be one of the main reasons of the low critical exponent of yield stress. This speculation needs to be investigated further by comparing with models of more regular structures, such as homogeneously packed sand grains or mathematically created digital rocks.

3 CONCLUSIONS

- In this study we have established a workflow of upscaling of physical properties from microtomography. A carbonate sample is used to test the workflow. The sample is heterogeneous and performs as a case study. Mechanical RVE, plastic strength and the critical exponent of yield are three elements proving the applicability of the work flow.

- Mechanical RVE can be determined from the thermo-dynamical principle of upper and lower bounds for a series of models of different sizes. Lower bound (or constant force boundary condition) causes softer response but stronger oscillation than upper bound (or constant displacement boundary condition). As the volume size increases the upper and lower bounds give convergent results. The size of the mechanical RVE of this carbonate sample is 320-cube voxels. As the resolution is 2.9 $\mu$m, the physical size of the mechanical RVE is close to 1 mm$^3$.

- Plastic strength has been analyzed based on microstructures from microtomography for Drucker-Prager plasticity. By analyzing two responses of Drucker-Prager plastic behaviour under different pressures, cohesion and the angle of friction are obtained. The carbonate sample with 23.3% porosity has two-thirds of cohesion of the solid parameter, and its angle of friction has reduced to around one-third of the solid parameter. This re-
result is the first step to establish a relationship of porosity and plastic strength. More numerical simulations and laboratory experiments are necessary to specify this relationship.

- The critical exponent of the yield strength has been extracted from the derivative models with different volume fractions close to the percolation threshold. This is the first test of rock samples using numerical simulations. The value we have got does not match the result of theoretical deduction and laboratory experiments very well. Whether it is caused by the strong heterogeneity of the structure needs more investigations. This is a valuable pilot study and it paves the road of research of upscaling of physical properties from microtomography of different materials.

ACKNOWLEDGEMENT

We are grateful to Petrobras’ support of this research. We thank Ali Karrech, Thomas Poulet, and Valeriya Shulakova in CESRE for their help on finite element computing and pre/post-processing. We also thank Ben Clennell and Thomas Poulet for their comments and suggestions to improve the manuscript.

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