Segmentation of 3D FIB-SEM data with pore-back effect

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Abstract. Digital rock physics is used for the investigation of oil and gas reservoirs. It involves various mathematical simulations on a digital representation of a rock sample, which is usually obtained with imaging techniques. Focused ion beam scanning electron microscopy (FIB-SEM) tomography provides high-resolution images of sequential layers of a sample, and segmentation of these images is a key stage in the construction of 3D digital rock. Conventional segmentation methods are not applicable for FIB-SEM images due to specific artifacts such as the pore-back effect. We propose a new segmentation algorithm that relies on the marker-controlled watershed, variance filter and morphological operations. The results are validated with the use of manually labelled ground truth data. Furthermore, we develop a new metric for evaluation of segmentation quality. This metric is based on analysis of segmented regions and, in the case of porous media, provides more reliable evaluation than pixel-wise measures.

1. Introduction

The oil and gas industry employs a wide range of scientific methods for hydrocarbon exploration, extraction and production. These include seismic, electromagnetic, and gravimetric surveys; well logs; transient pressure testing; digital rock physics; reservoir performance; and cores and drill cuttings. Digital rock physics includes mathematical simulations of liquid flows in porous media and numerically solving transport equations on digital representations of rock samples (i.e., “digital rock”) [1], [2]. This enables evaluation of the porosity, permeability and strength characteristics of a reservoir.

Generally, digital rock is constructed from X-ray microtomography images with resolution up to several micrometers. Another option is FIB-SEM tomography, which resolves details on the scale of about 5 to 10 nm and, therefore, provides more precise data about the interior structure of a sample. This technology is widely used in various fields including the semiconductor industry, materials science, and biology.

FIB-SEM tomography is a destructive serial-section technique and requires specific laboratory equipment. The principle is based on the combined operation of a focused ion beam (FIB) and scanning electron microscope (SEM) (see figure 1). Accelerated metal ions hit the sample and sputter atoms from its surface, thus removing a thin layer of substance. Then the electron microscope scans the surface and forms the image [3]. Multiple repetition of these two procedures produces a stack of sequential images that correspond to the sample slices.
FIB-SEM tomography not only implies visual analysis of materials structure, but also involves image processing to enhance the image quality, get further information of the samples (e.g., grain- and pore-size distribution) and construct a 3D digital rock. However, construction of a 3D model from a series of 2D FIB-SEM images must overcome some problems. The so-called pore-back or shine-through effect is a major obstacle to precise segmentation. This artifact arises when structures lying below the milling plane are visible through transparent pores and have similar intensity to the mineral matrix in the current slice (see Figure 2). Thus, during automatic image processing, a void phase is often confused with a solid one, and this leads to false segmentation [5].

Another related issue concerns evaluation of segmentation quality in case of porous media. In our opinion, simple pixel-wise metrics cannot assess segmentation algorithms properly because pore geometry and connectivity are as important as total pore volume.

In this paper, we propose a new method for segmentation of FIB-SEM images considering the pore-back effect and introduce a metric for the evaluation of segmentation quality. The paper is organized as follows. Section 2 gives a quick overview of the prior art, and in section 3, we describe the segmentation algorithm. Section 4 is devoted to the quality evaluation, and in section 5, we present our results on a real sample.

2. Related works

2.1. Existing algorithms for segmentation of FIB-SEM images

Although the pore-back effect is often mentioned as an obstacle to correct segmentation of FIB-SEM images, only few authors try to develop specific approaches [4]-[7]. Most of them do not simply rely on consecutive segmentation of 2D slices but process the entire 3D image or even focus on intensity changes along the z-direction. This axis is perpendicular to the milling plane (xy), and the coordinate corresponds to a slice number (see Figure 1).

Jørgensen et al. [4] introduce an algorithm based on an active contours approach [9] and use level set methods [10] to both evolve and represent the segmentation boundary. Voxel misclassification rate (false positives and false negatives) and segmented porosity area serve as segmentation metrics for FIB-SEM images of solid oxide cell materials.

A local threshold backpropagation is developed by Salzer et al. [5]. It compares gray values in the z-direction and detects the appearance and disappearance of structures based on this comparison rather than relying on absolute gray values. The algorithm finds considerable local minima and regards them as the end of solid phase. Then it estimates a reasonable local threshold from the last slice just before the corresponding substructure was cut off. These thresholds are then backpropagated to earlier slices.
The results are demonstrated on FIB-SEM images of a synthetic highly porous silicate material which is completely different from the porous structure of oil-bearing rocks.

Further extension of this approach is introduced in [6]. The authors attempt to detect the first and last occurrences of individual structures by selecting salient local minima and maxima respectively, i.e., finding a “valley” in gray values along z-axis. The algorithm is applied to FIB-SEM images of cathode material used in polymer electrolyte membrane fuel cells. The results are validated by comparison with manual segmentation in terms of misclassification rate and spherical contact distribution function.

Prill et al. [7] investigate the structure of a carbon-based negative Li-ion battery electrode and use the marker-controlled watershed transformation [11]. The main problem of such approach is to find correct markers of solid and void phases. Figure 3 briefly illustrates the procedure. The first step is extraction of dark regions that correspond to deep pores, so \( F_{GV} \) is the result of low-value thresholding. Second, peaks of morphological gradient \( F_{Grad} \) [12] are located on the edges of regions with different intensities. Third, reconstruction by dilation [13] keeps only considerable minima, i.e., having the dynamics (or amplitude) not less than some predefined value. Using a hit-or-miss transform, the first pixels of these minima are found, and the result is denoted by \( F_{min} \). Thus, \( F_{min}^{(2)} \) which is the intersection of \( F_{Grad} \) and \( F_{min} \) contains pixels of pores that appear immediately after the solid structure has been cut off. Fourth, the morphological half-gradient by dilation \( F_{halfgrad} \) is thresholded to find homogeneous regions corresponding to mineral matrix. The result of the operation is denoted by \( F_{Art} \). Then, \( F_{Seg} \) is reconstructed by dilation with the marker image \( F_{Art} \) and the mask that equals \( \text{NOT} (F_{min}^{(2)} \cup F_{GV}) \). In other words, \( F_{Art} \) “grows” up to beginning of pores, so in the first approximation, \( F_{Seg} \) represents slightly extended matrix markers. Finally, eroded \( F_{Seg} \) serves as matrix markers \( F_{Matrix} \), and pore markers \( F_{Void} \) are found as the sum of erosions of \( F_{GV} \) and negative \( F_{Seg} \). Watershed transformation is applied to morphological gradient \( F_{Grad} \). Validation was done for synthetic data by the same criteria as in [8].

Paper [8] analyzes segmentation of algorithms described in [5]-[7] using synthetic data. They are compared based on the error for the estimated volume fraction, the number of misclassified voxels, covariance function and granulometry by openings. As concluded from the results, the choice of specific method strongly depends on the type of the studied sample and its porosity.

Another method intended for segmentation of FIB-SEM images is presented in documentation of Avizo software (Thermo Fisher Scientific, USA). It is also based on the marker-controlled watershed algorithm but employs a slice-by-slice approach [14]. Low-value thresholding and a morphological operation both [12] find dark regions in the image and, therefore, extract pore markers. Then, a variance filter [15] with kernel size from 15 to 25 pixels is applied to highlight regions with nonuniform intensity. Thresholding of the result produces markers of for the solid phase, which is supposed to be homogeneous. Because large pores can also have uniform gray values, it is recommended to find matrix markers first and then “rewrite” pixels as pores in case of collisions. We suppose slice-by-slice (2D) processing combined with the described method of pore detection makes the approach unreliable. The reason is that a pore often begins in previous slices, so the current slice lacks for pores markers.

2.2. Metrics used for evaluation of segmentation quality

From the previous subsection, the volume fraction, the number of misclassified voxels, covariance function and granulometry by openings are frequent quality metrics used for assessment of segmentation of FIB-SEM images [4]-[7]. Jørgensen et al [4] note that the volumetric characteristics are not reliable because the corresponding error is equal to zero when the number of false positives and false negatives are equal. The number of misclassified voxels is not suitable in case of porous media either.

Pont-Tuset and Marques [17] analyze various criteria of segmentation quality. Precision, i.e., part of correctly segmented pixels, is one of the simplest pixel-wise criteria. The Jaccard index is another popular criterion. It is often referred to as intersection over union (IoU) between the machine and the
ground truth results. In [16], global consistency error and the Rand index are employed to evaluate segmentation of hyperspectral images.

A multiclass segmentation measure was used by Antonacopoulos et al. [18] in the document segmentation competition for the International Conference on Document Analysis and Recognition (ICDAR) in 2007. This measure is based on the concept proposed by Phillips and Chhabra [19] for estimation of recognition quality of several primitives of vector graphics such as lines, circles and arcs. We suppose this criterion can be adjusted for region-wise assessment of segmentation quality in our problem.

![Segmentation Workflow Diagram](image)

**Figure 3.** A scheme of the segmentation workflow developed by Prill et al. [7].

3. Segmentation method
Before we describe the proposed algorithm, let us consider how intensity changes as slices are cut off. Most pores begin with small dark regions. Then, a pore is gradually “opened”, becomes brighter and then ends (Figure 4).
Figure 4. A pore in different slices in (xy)-plane.

It is also useful to look at side view of 3D image, i.e. iterate through 2D slices not only in the original (xy)-plane as in Figure 4, but also in two other planes (xz) and (yz). Figure 5 demonstrates an intensity profile taken from the side view of a FIB-SEM image and a plot of intensity versus slice number for some fixed position (x, y). The mineral matrix corresponds to rather stable gray values and pores correspond to nonuniform intervals beginning from sharp drops.

Figure 5. An intensity profile on side view.

As seen from Figure 5, intensity changes are hardly greater than noise level at the points when the void phase is changed by the solid one. We suppose that watershed algorithm can be used to build the missing border. The proposed algorithm employs a 3D approach, so all operations affect the whole set of slices. Noise elimination and alignment must precede segmentation. We apply a bilateral filter to suppress noise and to preserve edges between regions with different intensities [20]. Alignment is done by the Image Stabilizer plug-in [21] developed for open-source software ImageJ [22], [23].

As mentioned before, voxels of mineral matrix have almost the same gray value on average. A 3D variance filter [15] given by equation (1) enables finding these homogeneous regions. Thresholding of the result (3) produces the markers of the solid phase (Figure 6).

\[ f_{\text{var}}(x, y) = \frac{1}{W^2} \sum_{i=0}^{W-1} \sum_{j=0}^{W-1} \left( f(x + i, y + j) - \frac{W}{2} \right)^2 \]

(1)
where [ ] takes integer part, \( W \) is window size, \( f(x,y) \) is intensity of pixel at \((x,y)\) position, \( x = \left\lfloor \frac{W}{2} \right\rfloor \ldots (N - \left\lfloor \frac{W}{2} \right\rfloor - 1) \), \( y = \left\lfloor \frac{W}{2} \right\rfloor \ldots (M - \left\lfloor \frac{W}{2} \right\rfloor - 1) \), \( N \) and \( M \) are numbers of the image rows and columns, respectively, and the expected value \( \bar{f}_W \) is given as

\[
\bar{f}_W(x,y) = \frac{1}{W^2} \sum_{i=0}^{W-1} \sum_{j=0}^{W-1} f \left( x + i - \left\lfloor \frac{W}{2} \right\rfloor, y + j - \left\lfloor \frac{W}{2} \right\rfloor \right)
\]  

For the further steps, we need to introduce some morphological operations. Half-gradient by erosion \( G_E \) is the difference between the original and eroded image \( E(f) \) and half-gradient by dilation \( G_D \) comes from subtraction of the original image \( f \) from dilated one \( D(f) \):

\[
G_E(f) = f - E(f),
\]
\[
G_D(f) = D(f) - f.
\]

Both half-gradients highlight voxels situated near the edges between the regions with different intensities, but in case of dilation, these voxels belong to the darker region and in case of erosion, they belong to the lighter one (Figure 6). Based on this, pore markers are produced by thresholding of original image \( f \) and its half-gradient by dilation \( G_D(f) \) with values \( T \) and \( T_{\text{hg}} \), respectively:

\[
f_{\text{pores}} = (f < T) \text{ or } (G_D(f) > T_{\text{hg}}).
\]

There are several options for watershed relief. We used the sum of the original image and half-gradient by erosion. The zero-crossing of the Laplacian of Gaussian (LOG) edge detector and the morphological gradient are the alternatives of the half-gradient. Figure 7 demonstrates the entire workflow.

4. Segmentation criteria
We suppose that pixel-wise metrics do not match the problem of assessment of segmentation quality in the case of porous media because pore shape and connectivity are as important as pore size. Besides that, a pixel-wise measure works well only in the case of ideal ground truth, but FIB-SEM images contain many uncertainties and are always segmented differently by different experts. Thus, a pixel-
wise quality criterion unfairly “fines” even quite good algorithms if they make minor mistakes on region edges. Moreover, small but important regions (for example, in case of low-porosity rock) do not contribute significantly in the final score. Therefore, region-wise criteria are preferable.

In this section, we propose a new segmentation measure based on ideas from [18] and [19]. We introduce the following designations illustrated in Figure 8:

- $G$ is the image that sets pore pixels in the ground truth (or reference) image equal to 1, and other pixels equal to zero;
- $S$ is the same towards segmented image;
- $N$ and $M$ are the numbers of connected regions in $G$ and $S$, respectively;
- $g_i$ is the $i^{th}$ connected region in $G$, $i = 1…N$;
- $s_j$ is the $j^{th}$ connected region in $S$, $j = 1…M$;
- $G_s_j$ is a set of those connected regions in $G$ that have non-empty intersection with the region $s_j$, i.e. $G_{s_j} = \{g | g \in G, g \cap s_j \neq \emptyset\}$;
- $S_{g_i}$ is a set of connected regions in $S$ that have non-empty intersection with $g_i$, which means $S_{g_i} = \{s | s \in S, s \cap g_i \neq \emptyset\}$;
- $n(x)$ counts number of non-zero elements in image $x$.

For each region $g_i$ and $s_j$ we calculate intersection over union $GIOU_i$ and $SIOU_j$, respectively:

$$GIOU_i = \frac{n(g_i \cap S)}{n(g_i \cup S_{g_i})}$$  \hspace{1cm} (7)

$$SIOU_j = \frac{n(s_j \cap G)}{n(s_j \cup G_{s_j})}$$  \hspace{1cm} (8)

Relying on these values, we distinguish three cases of correspondence of regions in segmented and ground truth images (see Figure 8). In the case of one-to-one correspondence, one segmented region $s_j$
stands for one region of reference (i.e. \( s_j \cap G \) contains only one connected region) and \( SIOU_j \) is bigger than some predefined threshold: \( SIOU_j > \text{thresh} \). One-to-many means that one segmented region \( s_j \) corresponds to several regions from ground truth image (\( s_j \cap G \) contains more than one connected region) and \( SIOU_j > \text{thresh} \). Finally, many-to-one is when several segmented regions correspond to one region of reference (\( g_i \cap S \) contains more than one connected region) and \( GIOU_i > \text{thresh} \).

Figure 8. Ground truth (solid blue line) and segmented (dashed red line) slices.

Then, we calculate numbers of these cases: one-to-one \( n_{OO} \), one-to-many \( n_{OM} \) and many-to-one \( n_{MO} \). Detection rate \( DR \) and recognition accuracy \( RA \) are defined as:

\[
DR = \frac{w_1 n_{OO} + w_2 n_{OM} + w_3 n_{MO}}{N},
\]

\[
RA = \frac{w_4 n_{OO} + w_5 n_{OM} + w_6 n_{MO}}{M},
\]

where \( w_i \) are weights which allow to adjust relative importance of cases. We use the same weights as in [18] to give maximum score to one-to-one matches: \( w_1 = w_4 = 1, w_2 = w_3 = w_5 = w_6 = 0.75 \).

Final segmentation metric \( RM \) is calculated as a harmonic mean of \( DR \) and \( RA \):

\[
RM = \frac{2 DR \times RA}{DR + RA}.
\]

For a 3D image, we calculate this measure slice-by-slice and then average it. The reason is that in the case of enough volume, almost all pores are connected to each other, and we get one connected region. We also calculate the accuracy and the Jaccard index:

\[
\text{Accuracy} = \frac{n(G \cap S)}{n(G \cup \bar{G})}
\]

\[
\text{Jaccard Index} = \frac{n(G \cap S)}{n(G \cup S)}
\]
5. Results

We manually labelled a set of 150 images with size 200×250 pixels and used them as ground truth. Our method, as well as the Avizo and Prill et al. [7] algorithms, were implemented with Python. The following parameters were used:

- bilateral filter from OpenCV library [24]: \( d = 11, \sigma_{\text{Color}} = 20, \sigma_{\text{Space}} = 30 \);
- Avizo algorithm: threshold for pore markers \( \text{threshold}_{\text{pore}} = 110 \), size of structure element for both that \( \text{connectivity}_{\text{both}} = 9 \), threshold for both that \( \text{threshold}_{\text{both}} = 25 \), kernel size for variance filter \( \text{window}_{\text{variance}} = 15 \), threshold for variance filter \( \text{threshold}_{\text{variance}} = 4 \), standard deviation for LOG \( \sigma_{\text{LOG}} = 3 \);
- Prill et al. [7] algorithm: threshold for pore markers \( \text{threshold}_{\text{pore}} = 110 \), threshold for morphological gradient \( \text{threshold}_{\text{morphgrad}} = 20 \), minimum dynamics \( d_{\text{min}} = 30 \), threshold for half-gradient by dilation along z-axis \( \text{threshold}_{\text{halfgrad, dil, z}} = 2 \), size of structure element for half-gradient \( \text{connectivity}_{\text{halfgrad}} = 15 \);
- the proposed algorithm: threshold for pore markers \( \text{threshold}_{\text{pore}} = 110 \), size of structure element for half-gradients \( \text{connectivity}_{\text{halfgrad}} = 7 \), threshold for half-gradient by dilation \( \text{threshold}_{\text{halfgrad, dil}} = 60 \), kernel size for variance filter \( \text{window}_{\text{variance}} = 15 \), threshold for variance filter \( \text{threshold}_{\text{variance}} = 4 \).

Ground truth and the results of segmentation by various algorithms are demonstrated in Figure 9. As Figure 9b shows, 2D processing of the 3D image results in an improper segmentation that cannot be used for liquid flow simulations. The second algorithm (Figure 9c) is better, but there are mistakes in the first slices. The outcome of proposed segmentation technique looks admissible.

We calculated segmentation quality for all three methods in terms of \( \text{Accuracy} \) (12), \( \text{Jaccard Index} \) (13) and averaged-by-slices region-wise metric \( \text{RM}_{\text{avg}} \) (11). Table 1 contains estimations of segmentation quality. Despite visual evidence that the proposed algorithm works better, its score by \( \text{Accuracy} \) is a little lower in comparison with Prill’s approach. This illustrates once again that pixel-wise metrics are ineffective for our problem. Two other indices gave the maximal score to the proposed algorithm.
Table 1. Estimation of segmentation quality.

|                | Accuracy | Jaccard Index | Averaged region-wise metrics |
|----------------|----------|---------------|----------------------------|
| Avizo algorithm| 0.87     | 0.47          | 0.09                       |
| Prill et al. [7]| 0.90     | 0.53          | 0.22                       |
| Proposed method| 0.89     | 0.57          | 0.25                       |

6. Conclusion

We proposed an approach for segmentation of FIB-SEM images of rocks, which is the key stage in the reconstruction of 3D digital rock from 2D slices. We validated the results by several measures of segmentation quality with the use of manually labeled images of a real rock sample. Our algorithm outperforms two existing methods in segmentation of middle-porosity rocks, but the results are still far from perfect. One of the reasons is uncertainties of ground truth due to slight gradients on borders between solid and void phases, which complicate manual labelling. On the other hand, the algorithm should also be improved, especially in case of non-monomineralic matrix. For example, superpixel approach [25], [26] is often used to improve the performance of watershed algorithm.

In addition, we developed a region-based metric for evaluation of segmentation quality. We suppose that the proposed measure better describes segmentation of porous media because it relies on characteristics of segmented regions rather than on the number of correctly classified voxels.

7. References

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