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# Geometry segmentation of voxelized representations of heterogeneous microstructures using betweenness centrality

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ABSTRACT

We present a robust method for automating removal of "segregation artifacts" in segmented tomographic images of three-dimensional heterogeneous microstructures. The objective of this method is to accurately identify and separate discrete features in composite materials where limitations in imaging resolution lead to spurious connections near close contacts. The method utilizes betweenness centrality, a measure of the importance of a node in the connectivity of a graph network, to identify voxels that create artificial bridges between otherwise distinct geometric features. To facilitate automation of the algorithm, we develop a relative centrality metric to allow for the selection of a threshold criterion that is not sensitive to inclusion size or shape. As a demonstration of the effectiveness of the algorithm, we report on the segmentation of a 3D reconstruction of a SiC particle reinforced aluminum alloy, imaged by X-ray synchrotron tomography.



## 1. Introduction

The experimental techniques for characterizing a material's microstructure in three dimensions include atom probe tomography [1], electron tomography [2], serial sectioning followed by optical microscopy [3,4], and X-ray tomography [5,6]. Among these, 3D atom probe tomography provides resolution at the atomic detail, but as a result, only very small volumes can be analyzed. Serial sectioning techniques can analyze larger volumes, also at relatively high resolution, however these techniques are extremely time consuming and are destructive. In contrast, X-ray tomography can be used to analyze a significantly larger volume of a material, providing statistically significant information at typical resolutions of 1 μm, and recent advances have enabled resolutions of tens of nanometers to be achieved [7]. X-ray tomography is particularly attractive as it is a non-destructive technique requiring minimal sample preparation [8], and thus has been applied to characterize microstructural evolution during deformation in materials such as metal matrix composites [9] and Sn-based solders [10].

Due to limited resolution in X-ray tomography, it can be difficult to distinguish between different particles or inclusions in close proximity. As a consequence, neighboring but otherwise separate particles may erroneously appear to be connected. These artificial connections will not generally affect computations of average composite properties, such as the elastic moduli, that depend primarily on the volume fractions of the constituent phases. They may, however, have a strong influence on properties sensitive to extreme values, such as fatigue strength and fracture toughness, which are sensitive to particle clusters and/or the overall spatial distribution of particles [11]. In damage evolution simulations, narrow volumes formed by spurious connections will be a point of artificially high stress concentration that may lead to predictions of cracks at reduced loads or fewer cycles than would occur in the actual microstructure. To improve strength predictions, geometry segmentation of the tomographic data is needed to remove these spurious bridges connecting discrete particles. Moreover, as the capabilities and resolution of imaging technologies are rapidly improving, manual geometry segmentation is becoming increasingly cumbersome and infeasible. Thus, the objective of this work is to develop a robust algorithm for geometry segmentation of material microstructure from tomographic image datasets.

We first briefly summarize the current capabilities of geometry segmentation. Ketcham developed the BLOB3D computer code to separate contacting objects in X-ray tomography data of geological specimens [12]. BLOB3D uses the watershed algorithm [13] to separate objects in grayscale images, and erosive operations to remove connective volumes. Proussevitch developed an improved erosion scheme to separate individual convex objects by peeling away sequential layers of voxels until narrow bridges disappear [14]. In general, erosion methods are most effective for convex shapes with aspect ratios near unity. Zhong

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proposed a segmentation algorithm extending the watershed algorithm to further segment images using local concavities in order to identify slender particles [15]. This method, however, was only implemented in two dimensions, and relies on a-priori knowledge about the shape of the particles.

More generally, geometry segmentation can be thought of as a clustering or partitioning problem, and thus as context for this work, we present a brief survey of partitioning algorithms. Common algorithms for partitioning include k-means clustering [16], hierarchical clustering schemes [17], and density-based clustering methods [18,19]. K-means clustering is a distance-based approach that partitions a dataset of elements into clusters while minimizing the distances to the centroid of the cluster to which they belong. A major drawback of k-means clustering is that the number of clusters is an input to the algorithm, and thus for partitioning microstructural information, diagnostic checks may be required to estimate and update the number of particles in a voxel dataset. Furthermore, the k-means algorithm is optimal for spherical clusters of similar size, and thus, erroneous clusterings can be generated when particles have large aspect ratios or non-convex geometry [20]. In hierarchical clustering schemes, clusters of elements are either merged or split based on a measure of distance or similarity between each pair of elements until a threshold is met. The weakness of such an approach is that the matrix of element distances scales as the square of the number of elements, in the present case, the number of voxels within a phase. Density-based clustering is a more recent approach that groups together points that are closely packed together, utilizing local point densities to identify points as internal to clusters, outliers, or boundaries of clusters. Although density-based clustering approaches do not require one to specify the number of clusters and can find arbitrarily shaped clusters, the method is not deterministic in that the results are dependent on the starting point.

In this work, we develop a new method for geometry segmentation based on the concept of betweenness centrality [21], a measure of the importance of a node in a graph network. More specifically, the betweenness centrality is the fraction of shortest paths between nodes in a network that traverse a given node [22]. The centrality concept has been applied in various problems, including ecological studies of pollination networks [23], network mapping of the human brain [24] and biological studies of protein networks [25]. In the context of geometry segmentation, we test how well the betweenness centrality can serve as a metric for identifying artificial connections between nearly touching particles in segmented images. As betweenness centrality measures connectivity rather than position, our method bears similarities with density-based approaches. However, as the betweenness centrality is evaluated for all nodes in the network simultaneously, the method can be designed to be deterministic and does not depend on a starting position. Moreover, the centrality-based geometry segmentation is feasible for realistic networks containing millions of vertices due to the recently developed Brandes' algorithm [26]. Brandes' algorithm greatly reduces the effort required to compute the betweenness centrality for sparse graph networks with $O(VE)$ time complexity, where $V$ is the number of vertices and $E$ is the number of edges.

## 2. Methodology

In this section we describe a method for segmenting 3D voxelized microstructures for finite element simulations. For improved performance, the method is applied in several stages: a first pass that quickly segments non-contiguous voxel sets, which are then each segmented using the betweenness centrality measure, and then a final pass that enforces a minimum separation distance between discrete particles.

### 2.1. Centrality-Based Segmentation

The internal geometry of each phase within a heterogeneous material can be approximated by the set of voxels contained within the phase.

$$\mathcal{S}^{\alpha} = \{(i,j,k) : \mathbf{x}_{ijk} \in \Omega_{\alpha}\} \tag{1}$$

where $\Omega_{\alpha}$ denotes the subdomain containing phase $\alpha$, and each voxel is represented by a 3-tuple of integers. The location of each voxel is defined by:

$$\mathbf{x}_{ijk} = \mathbf{x}_0 + i\mathbf{a} + j\mathbf{b} + k\mathbf{c}, \tag{2}$$

where $\mathbf{x}_0$ is the origin of the domain, and $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ are the cell vectors connecting adjacent voxels.

Beginning with a voxel set defining a phase, an initial clustering step is performed to separate voxels into non-contiguous clusters. Voxels are considered contiguous if they share a face, but not if they share an edge or corner, i.e. in three dimensions, each voxel has only six connected neighbors. As a result of limited imaging resolution or poor contrast between adjacent particles, these initial sets of voxels often contain more than a single particle connected through artificial bridges. Geometry segmentation based on betweenness centrality is then applied to detect and eliminate these spurious connections.

After initially separating voxels into non-contiguous clusters, each set of clusters is analyzed to detect whether it is composed of a single particle or multiple particles connected by spurious bridges. For this purpose, we construct an unweighted, undirected graph network such that each voxel within a cluster is a node and edges are defined between all adjacent voxels. Fig. 1 illustrates the creation of graph networks for a domain containing two non-contiguous clusters. We note that the construction of the graph networks does not involve the physical coordinates of each voxel, but only the relative connectivity between voxels.

In order to identify voxels that form artificial bridges between particles, the betweenness centrality is calculated on each node of the constructed graph networks. The betweenness centrality is a metric that indicates the relative importance of a node in the connectivity of a network. In a graph with $V$ vertices, the betweenness centrality of vertex $v$ is defined according to Freeman [21] as:

$$g(v) = \sum_{s \neq t \neq v \in V} \frac{\sigma_{st}(v)}{\sigma_{st}}, \tag{3}$$

where $\sigma_{st}$ is the number of shortest paths between each vertex $s \in V$ and $t \in V$, and $\sigma_{st}(v)$ is the number of shortest paths passing through vertex $v$. The key concept is illustrated in Fig. 2, in which two particles are connected by a narrow bridge. As every path from voxels in particle 1 must traverse the voxels in the bridge to reach the voxels particle 2,

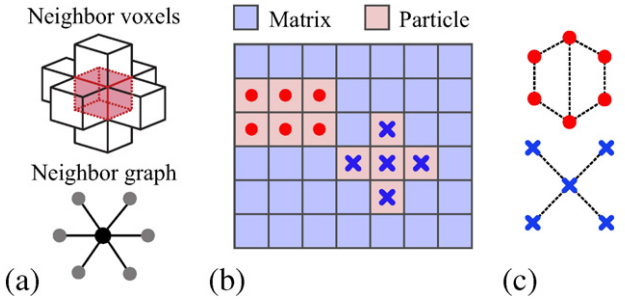


**Fig. 1.** Initialization of graph networks from phase voxel sets, (a) connectivity and graph of the neighbors around a single voxel, (b) example microstructure with two particles embedded in a matrix, (c) resulting graphs constructed from contiguous sets of particle voxels.