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Quantifying the effect of 3D spatial resolution on the accuracy of microstructural distributions

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Abstract

The choice of spatial resolution for experimentally-collected 3D microstructural data is often governed by general rules of thumb. For example, serial section experiments often strive to collect at least ten sections through the average feature-of-interest. However, the desire to collect high resolution data in 3D is greatly tempered by the exponential growth in collection times and data storage requirements. This paper explores the use of systematic down-sampling of synthetically-generated grain microstructures to examine the effect of resolution on the calculated distributions of microstructural descriptors such as grain size, number of nearest neighbors, aspect ratio, and Ω_3.

Keywords

microstructure, 3D characterization, serial sectioning, grain size

Introduction

Three dimensional (3D) microstructure characterization techniques are required to measure many important microstructural characteristics including true size and shape, the number of features per volume, and feature connectivity [1]. Although the need for 3D characterization for 'complete' microstructural analysis is well known, it is only within the past decade that desktop computing resources—such as processor speed, memory, graphics cards, and 64-bit operating systems—have advanced to the point where materials scientists and engineers are able to readily work with the enormous data sets born of 3D characterization experiments. These aforementioned advancements in computing technology have also helped galvanize activity in the materials community to promote and adopt Integrated Computational Materials Engineering (ICME) initiatives [2-4].

A foundational experimental technology for ICME-related research is the ability to quantify the internal material state at any point during the manufacturing or utilization of engineering materials, in order to verify and validate the output of modeling and simulation tools that examine such processes. This analysis ideally includes statistically-significant data on key microstructural features such as grains, precipitates, second phases, voids, and defects. Known capability gaps for this technology area include two topics related to 3D microstructure characterization; machines to rapidly collect 3D data across the range of lengths scales that are known to affect material properties [5], and computational methods to streamline the process of data reduction, analysis, and further re-use of data by other modeling and simulation tools. With the advent of new state-of-the-art 3D characterization systems that are addressing the need for rapid data collection, it is important to examine and investigate the sources of error associated with these characterization processes, in order to bound the uncertainty in quantitative measurements derived from such experiments.

In particular, there is little information in the materials characterization literature to guide the selection of sampling resolution for data collection in 3D. Prior guidance is particularly important for destructive experiments such as serial sectioning, where the sample volume is incrementally and irreversibly consumed during the experiment. In the serial sectioning literature, it is generally espoused that one would like a minimum of ten sections through a microstructural feature to accurately describe its size and shape, but this guidance is simply a rule-of-thumb and is wholly insufficient for quantitative microstructural analysis. Experimentalists can always strive to refine the spatial frequency of data collection, but this becomes problematic for 3D data when the collection times and storage requirements grow exponentially, often leading to considerable inefficiencies due to conservative oversampling.

This paper examines one aspect of modeling uncertainty with regards to 3D data collection, which is the effect that isotropic decrements in spatial resolution have on the accuracy of microstructural distributions that are derived from a reference data volume. Specifically, this work reports the quantitative change in the Hellinger Distance of the full distribution for the following morphological microstructure parameters: grain size in equivalent sphere diameter (ESD), grain shape as described by the two ellipsoid ratios *b/a* and *c/a*, the third moment invariant $\mathbf{\Omega}_3$ [6], and the number of contiguous neighbors. This analysis is performed for two near log-normal grain size distributions that have been synthetically-generated and virtually down-sampled, as described in the following section.

Methodology

The synthetic structure generation and subsequent data analysis for this study were performed using a state-of-the-art 3D materials analysis software DREAM.3D, or Digital Representation Environment for Analyzing Microstructure in 3D (dream3d.bluequartz.net). The 3D synthetic reference volumes were created using processes that are briefly described here; detailed reviews on synthetic microstructural generation methods have been reported previously [7].

The first step in the synthetic microstructure generation process is to define statistics that describe the grain size, grain shape, number of nearest neighbors, spatial orientation, crystallographic orientation and boundary character distributions for the desired volume. In this study, however, only morphological parameters are of interest and thus, the crystallographic orientation and boundary character distributions were omitted. Additionally, the number of nearest neighbors was not prescribed and was allowed to fluctuate as needed while placing the grains. Finally, the spatial orientation of the grains was assigned as random since the down-sampling was performed isotropically and not expected to be directionally sensitive. Two log-normal distributions were created for the reference grain size distributions and each volume was assigned a shape distribution that corresponded to roughly equiaxed grains. One of the grain size distributions was nearly uniform, which is termed 'slightly log-normal' ($\mu = 1.06$, $\sigma = 0.28$) while the other size distribution had a much heavier tail ($\mu = 0.95$, $\sigma = 0.55$), in order to examine the effect that the grain size distribution has on these uncertainty measurements of sampling frequency. After defining reference statistical distributions, grains are generated to fill the reference volume via random sampling of these distributions. The grains are then inserted into, removed from, or moved within the volume while optimizing a number of governing criteria (e.g., space filling, grain overlap, grain size and shape, and number of neighbors). After an optimal packing is obtained, a simulated coarsening process is used to eliminate unassigned voxels that remain from the inability to densely pack the reference volume with ellipsoids. The two synthetic reference volumes are shown in Figure 1A and 1B. Note that the reference volumes contain over 4000 grains (~2000 unbiased and used for analysis), and the spatial resolution for each volume is approximately 30 voxels through the diameter of a grain of mean size. Figure 1C shows the resultant grain size distributions of the two structures. Note that the reference distributions used to determine the effect of down-sampling are the distributions shown in Figure 1C, not the input distributions used to create the volumes.

To quantify the effect of data resolution, the two reference volumes were down-sampled using the following procedure. A new voxel volume was created using MATLAB at the desired down-sampling resolution. Voxels in the new volume were assigned a grain identification value that corresponded to the voxel in the reference volume in which their centroid fell. Successively coarser re-samplings of the reference synthetic microstructure volume were produced in this manner (i.e., the same reference volume was always used to assign the voxel grain identification of the down-sampled volumes), and the result of the down-sampling process is shown in Fig. 2.

The morphological parameter distributions examined in this study include grain size (ESD), grain shape (b/a, c/a, $\mathbf{\Omega_3}$), and number of neighbors. The ESD is computed using the following relation, where N_v is the number of voxels that comprise the grain, V is the voxel volume:

$$ESD = 2 \cdot \left(\frac{3}{4\pi} N_v V\right)^{\frac{1}{3}} \tag{1}$$

In this study, feature shape is described using aspect ratios of a best-fit ellipsoid and a second-order moment invariant (with respect to affine and/or similarity transformations) [6]. The moment invariant, denoted by $\mathbf{\Omega_3}$, is used to further describe grain shape and is calculated using the following equation [6]:

$$\Omega_3 = \frac{V^5}{O_3} \tag{2}$$

$$O_3 = \mu_{200}\mu_{200}\mu_{200} + 2\mu_{110}\mu_{101}\mu_{011} - \mu_{200}\mu_{011}^2 - \mu_{020}\mu_{101}^2 - \mu_{002}\mu_{110}^2 \tag{3}$$

where μ_{pqr} represents the second order moments in Eq. 3 (moment order is equal to the sum of *p, q* and *r*). $\mathbf{\Omega_3}$ can be used to differentiate shapes with the same aspect ratio, and shapes become qualitatively 'less complex' and more ellipsoidal-like with increasing values of $\mathbf{\Omega_3}$, up to the limiting case of $\mathbf{\Omega_3} = 2193.245$ that corresponds to spheres and ellipsoids [6]. In this study, all $\mathbf{\Omega_3}$ values have been normalized by that of a sphere to resultant in values bounded between 0 and 1.

The nearest neighbor distribution describes the number of grains that share at least one voxel face with a reference grain. Note that voxels which only share a common edge or corner are not considered as neighbor grains in this analysis.

Results and Discussion

The full distribution of grain size and Ω_3 for the 'heavy-tailed' structure at each down-sampling resolution is shown in Figs. 3 and 4, respectively. One can observe that the grain size distribution does not change markedly with down-sampling until there is nominally 1 voxel spanning the mean grain diameter. By comparison, the Ω_3 distribution is clearly affected by down-sampling even when there are as many as 20 voxels spanning the mean grain diameter. While this type of visual inspection can be informative, it is also useful to have metrics to characterize how the feature distributions are changing with down-sampling resolution. This study has used the Hellinger Distance (HD) to quantify the difference between two distributions, which is defined for discrete distributions as the following:

$$\mathrm{HD} = \sqrt{1-\sum_{i=1}^{n}\sqrt{R_i\,S_i}} \tag{4}$$

where R_i and S_i correspond to the data percentage in bin i for the discrete distributions R and S. The HD is used to measure the geometric similarity between two distinct statistical distributions (models), and is bounded between 0 and 1, where a value of 0 implies that two models are identically distributed. For this work, microstructure parameter data was binned into histograms after being computed from down-sampled and reference volumes. Therefore, the HD was computed discretely using a direct comparison of histograms over the entire domain of possible parameter values [8].

A plot of the statistical analysis of the down-sampled volumes from the slightly log-normal grain size distribution is shown in Fig. 5. At 20 voxels spanning the mean grain size, the HD for most of the feature distributions are nearly equal to 0, which indicates that there is very little difference in the measured distributions. However, the shape parameter Ω_3 is the most sensitive to resolution changes and requires significantly more sections through each feature to retain a low HD. This sensitivity is highlighted by the increase in the Ω_3 HD from 0.11 at 20 voxels spanning the mean grain size to 0.34 at 10 voxels and 0.75 at 5 voxels. Importantly, the grain size, ellipsoid ratios *b/a* and c/a, and nearest neighbor distributions continue to match the reference volume distributions (HD < 0.1) with progressively-coarser down-sampling to as low as 5 voxels spanning the mean grain size. This resolution is considerably less than the traditional rule-of-thumb of 10 sections through the average feature. However, for sampling resolutions below 5, all of the feature distributions begin to deviate rapidly from the reference distribution, as the shape & volume for the smallest grains in the distribution are becoming strongly altered by the relative coarseness of the voxel array.

A plot of the statistical analysis of the down-sampled volumes from the heavy-tailed grain size distribution is shown in Fig. 6. The global trends in the data are similar to the slightly log-normal distribution: Ω_3 is the most sensitive to changes in sampling resolution, and save for this parameter, all other distributions had HD values lower than 0.17 at 5 voxels spanning the mean grain size. Note that the heavy-tailed volume contains comparatively more small grains relative to the slightly log-normal volume. As a result, the microstructural distributions calculated from the heavy-tailed volume are affected first by changes in resolution, given that the smallest grains will be most altered by sampling resolution changes.

This study highlights the intrinsic effect of sampling resolution on the accuracy of microstructural distributions derived from 3D data. The virtual down-sampling experiments show that the probability distributions for grain size, number of neighbors, and ellipsoid ratio can be collected at relatively coarse resolutions with little alteration. Conversely, selected shape descriptors such as Ω_3 require high spatial resolution data. Although the methodology outlined herein has only been used to quantify one source of uncertainty, this method can be extended to examine many other sources data uncertainty, and will likely be especially effective with regards to improved analysis of destructive experimental methods like serial sectioning. For example, this approach could be used to optimize the selection of anisotropic sampling resolution (e.g., higher in-plane resolution relative to the sectioning depth), or examine the impact of variability within the serial sectioning process (planarity, parallelism, uniformity). While these concepts are not explored here and are left to future work, these types of studies should improve both data quality and experimental efficiencies.

References

[1] DeHoff, R.T., J. Microsc. 131 (1983) 259–263.
[2] Materials Genome Initiative for Global Competitiveness, June 2011
[3] Allison, J., “Integrated Computational Materials Engineering: A Perspective on Progress and Future Steps,” Journal of Materials, Vol. 63, No. 4, April, 2011, pp. 15-18.
[4] Christodoulou, J., “Dynamic 3D Digital Structure: Program Overview,” *Journal of Materials*, Vol. 61, No. 10, 2009, p. 21.
[5] Uchic, M.D., Groeber, M.A., and Rollet, A.D., “Automated Serial Sectioning Methods for Rapid Collection of 3-D Microstructure Data,” *Journal of Materials,* Vol. 63, No. 3, 2011, pp. 25-29.
[6] MacSleyne, J.P., Simmons, J.P., and De Graef, M., “On the use of moment invariants for the automated analysis of 3D particle shapes,” *Modelling and Simulation in Materials Science and Engineering*, Vol. 16, April, 2008,
[7] Groeber, M.A., *Computational Methods for Microstructure-Property Relationships,* ed. Ghosh, S., and Dimiduk, D. (New York: Springer, 2011), pp. 53-97
[8] Riley, M.E., and Grandhi, R.V., “Quantification of model form and predictive uncertainty for multi-physics simulation,” *Computers and Structures*, Vol. 89, Issues 11-12, June 2011, pp.1206-1213.

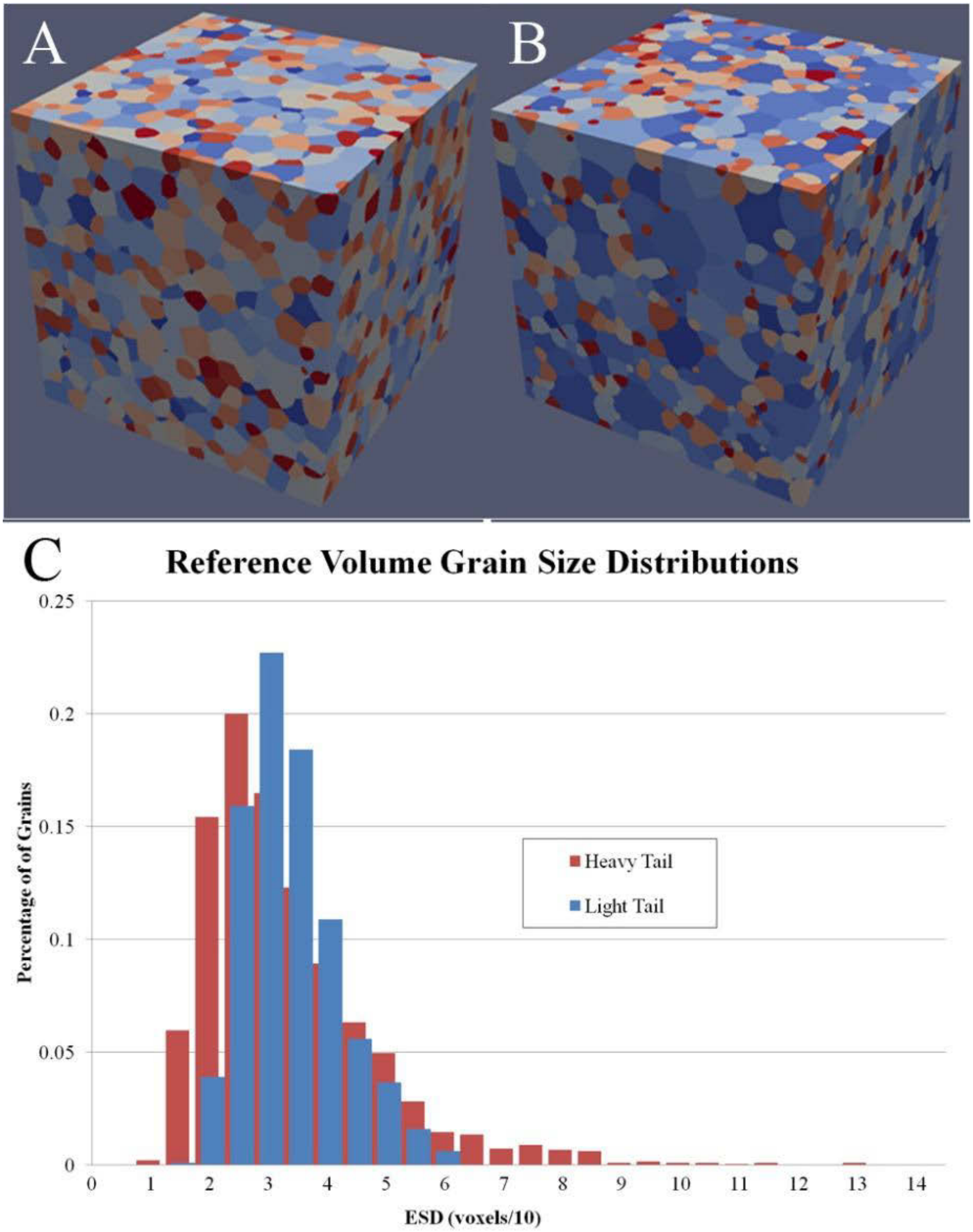

Figure 1: 3D renderings of the two synthetically-generated reference volumes. Panel A shows the slightly log-normal grain size distribution, while Panel B shows the heavy-tail grain size distribution. Grain coloring corresponds to unique grain IDs. Panel C plots the grain size distribution for the two volumes, and clearly shows that the heavy-tail volume has a greater number of both larger and smaller grains compared to the slightly log-normal volume.

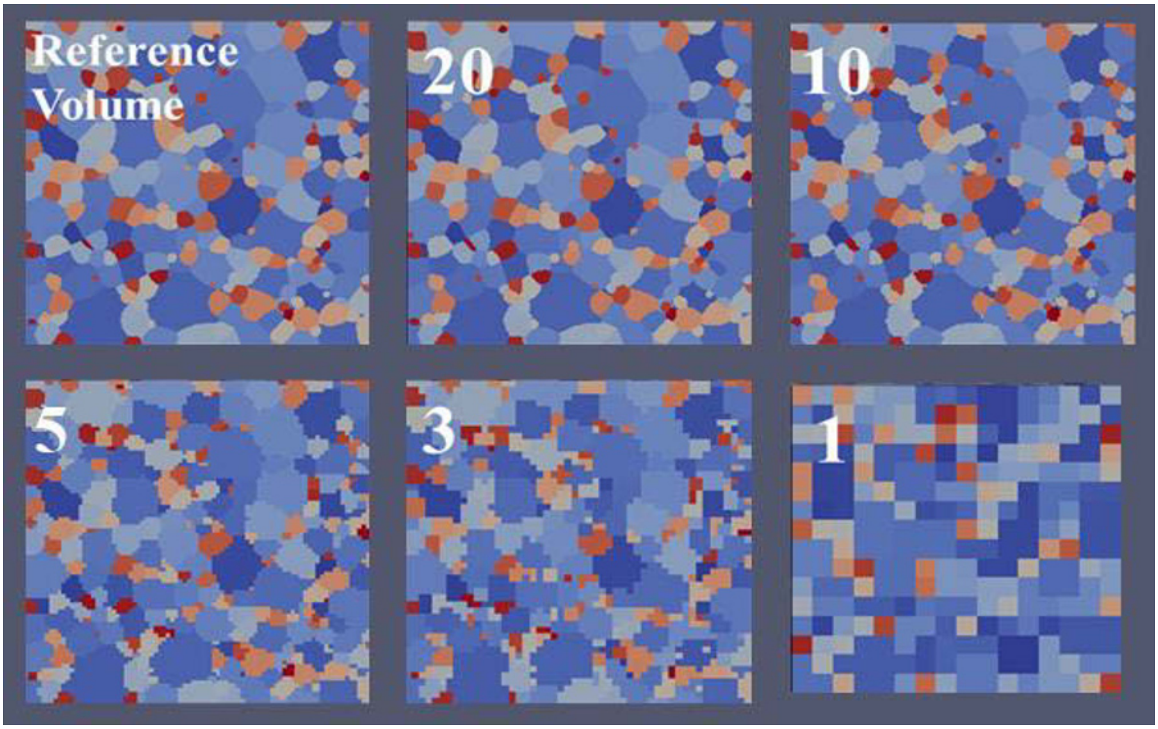

Figure 2: Images of successively down-sampled volumes for the heavy-tailed distribution. Spatial resolution is listed at the upper-left corner of each sub-image, which is defined as number of voxels that span the mean ESD.

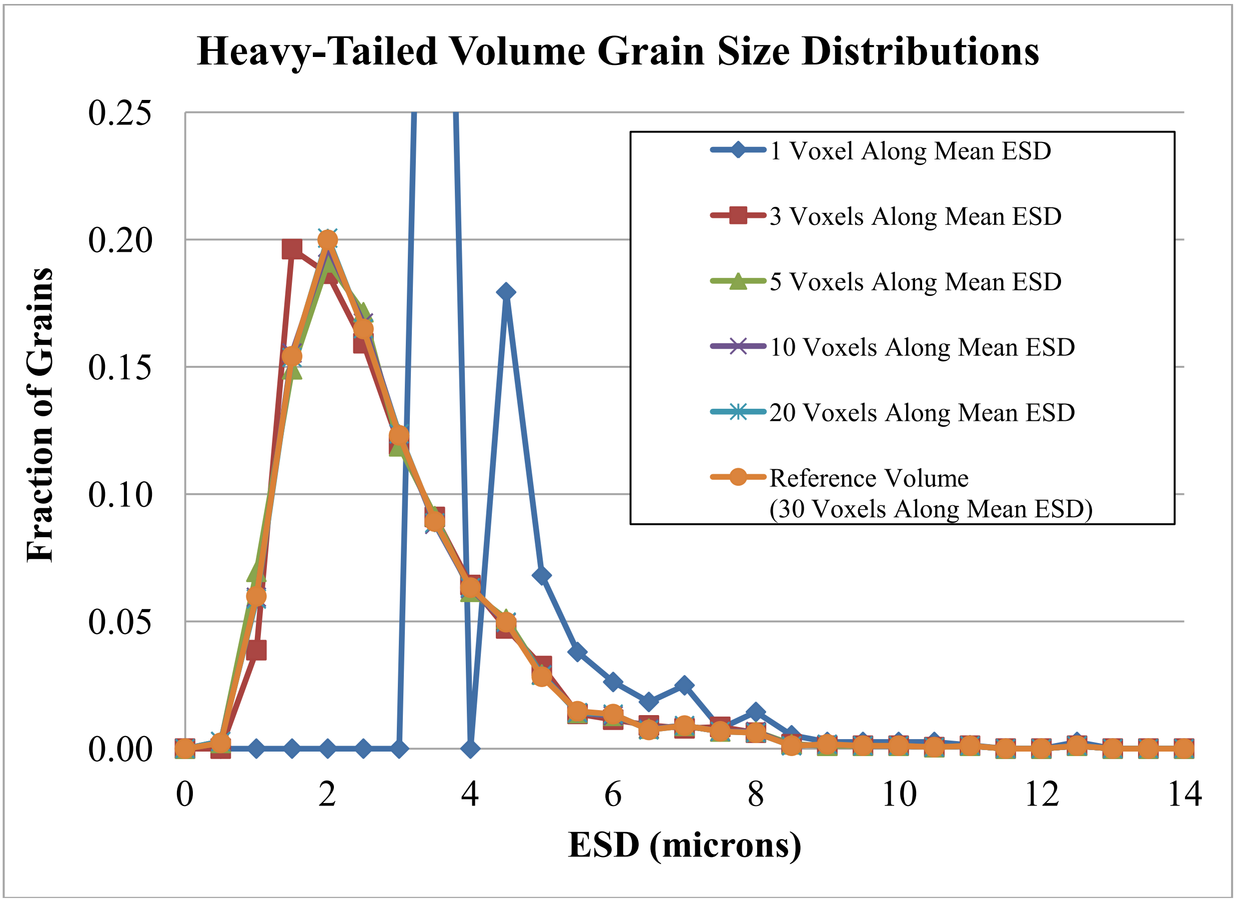

Figure 3: The effect of down-sampling from the reference volume on the ESD distribution is shown here for the heavy-tailed volume. Only minimal changes to the distribution are visible from down-sampling, until a down-sampling of 3 voxels along the mean ESD.

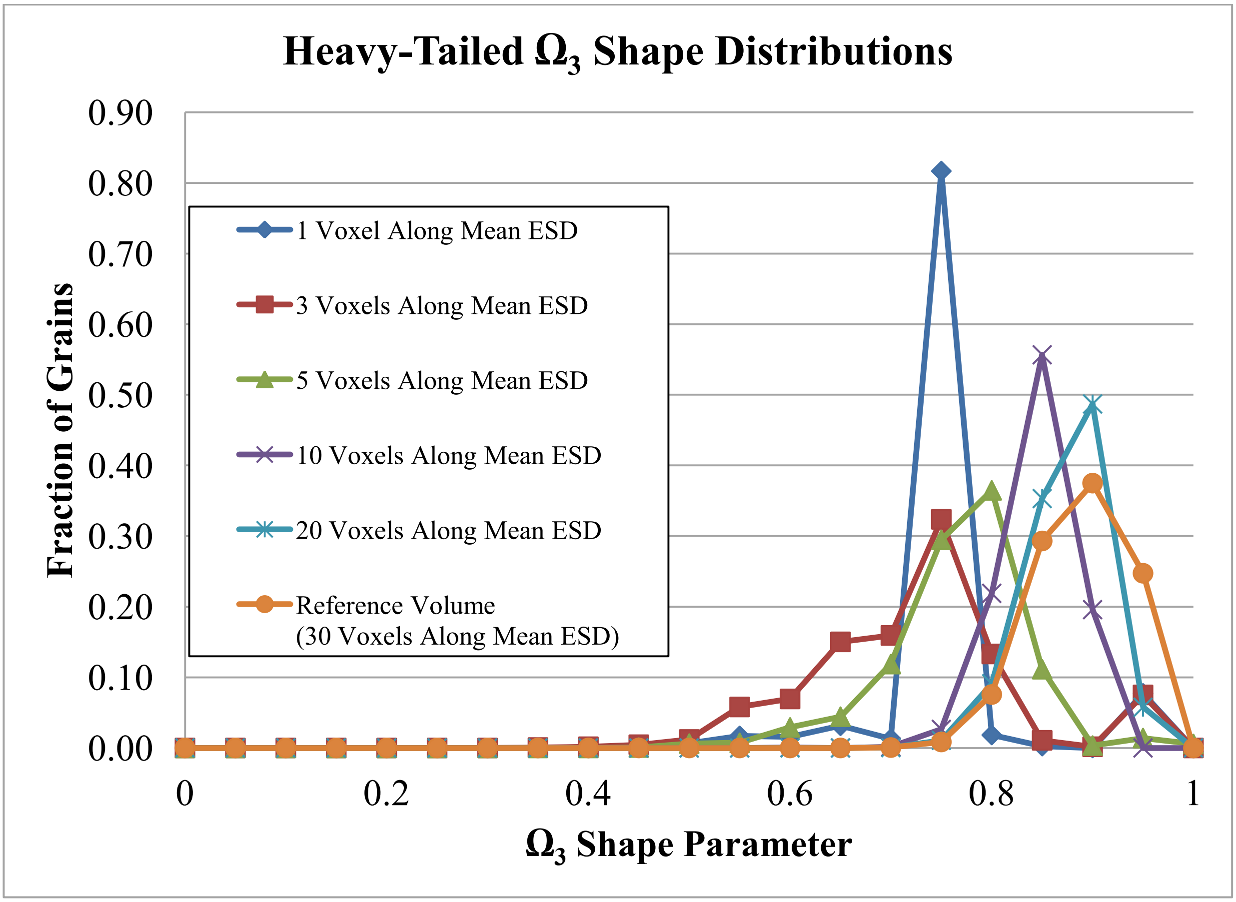

Figure 4: The effect of down-sampling from the reference volume on the Ω_3 distribution is shown here for the heavy-tailed volume. Changes in the distribution can be seen even at a down-sampling from 30 to 20 voxels along the mean ESD.

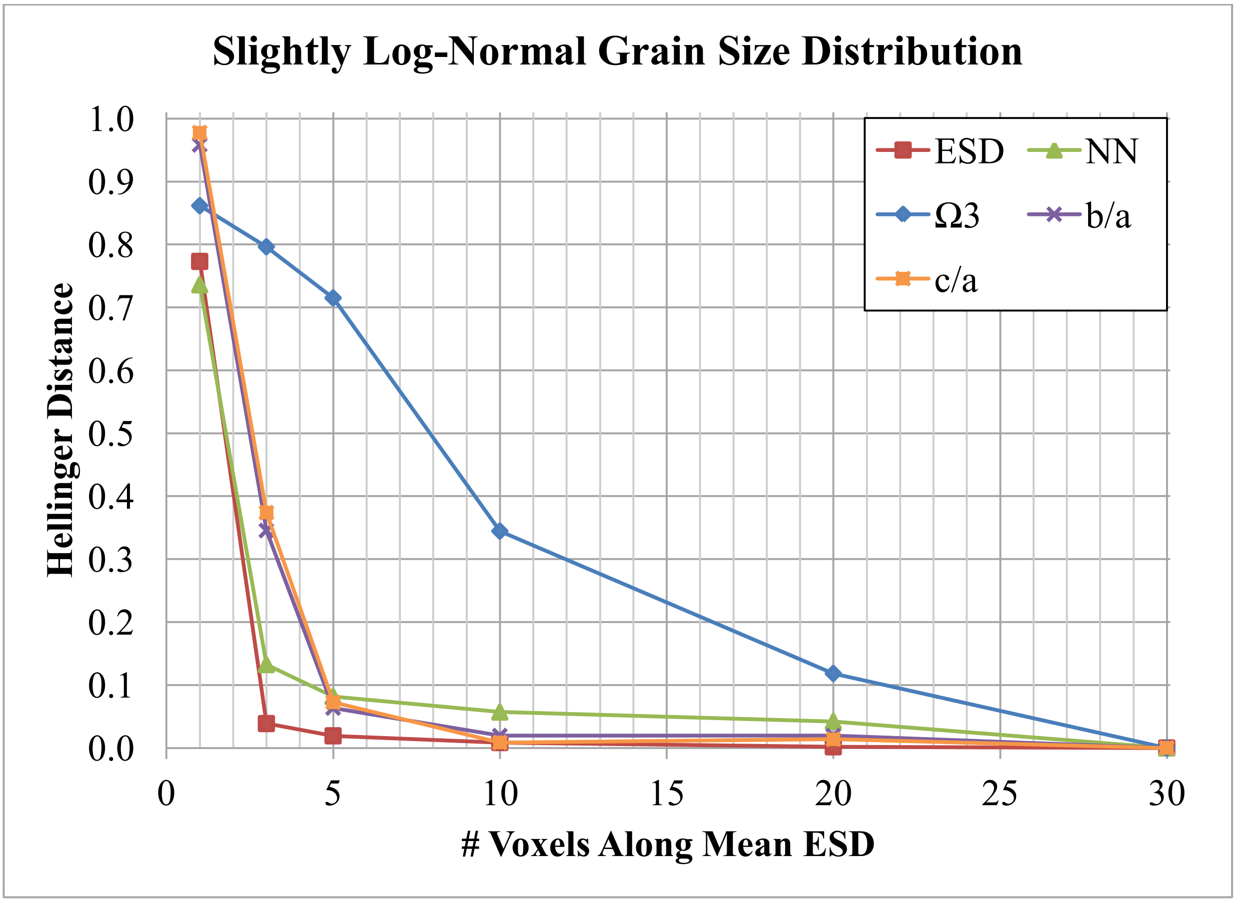

Figure 5:.The effect of down-sampling on the Hellinger Distance for slightly log-normal grain size distributions are illustrated here for ESD, NN, Ω_3, c/a and b/a distributions. The reference volume had 30 voxels along the mean ESD, and was down-sampled all the way to 1 voxel along the mean ESD.

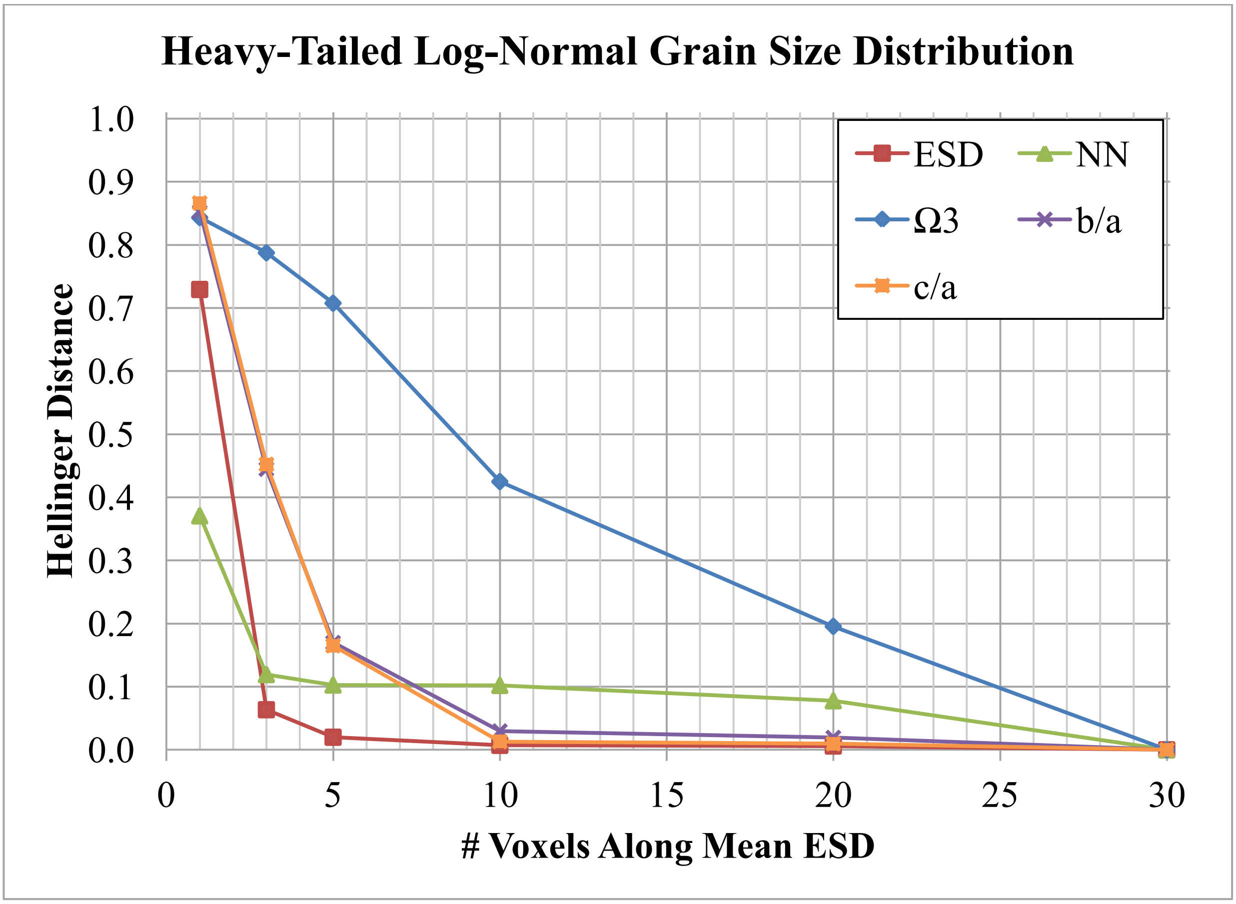

Figure 6: Plot of the Hellinger Distance relative to the number of voxels that span the mean ESD for the heavy-tailed log-normal grain size distribution. The effect of down-sampling on the Hellinger Distance for heavy-tailed log-normal grain size distributions are illustrated here for ESD, NN, $\Omega_{3,}$ c/a and b/a distributions. The reference volume had 30 voxels along the mean ESD, and was down-sampled all the way to 1 voxel along the mean ESD.