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IMPROVED MESOSCALE MATERIAL PROPERTY BOUNDS BASED ON VORONOI TESSELLATION OF STATISTICAL VOLUME ELEMENTS

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Abstract.

An important concern in mesoscale micromechanics is the accuracy with which material properties can be characterized at the mesoscale. These are scales that are smaller than the scale of the representative volume element (RVE), which is the scale at which material property behavior can be characterized independent of traction and displacement boundary conditions. In this work, to increase the accuracy with which randomly heterogeneous materials can be characterized at the mesoscale, the RVE is partitioned into statistical volume elements, (SVE), using Voronoi Tessellation. This approach is shown to have advantages over the use of square partitioning. The material property parameters generated by this approach are analyzed using the Principle of Maximum Entropy (MaxEnt) to create probability density functions (PDFs). These PDFs are compared for different cases of material contrast ratio, partition scheme, partition size, and microstructural morphology.

Key words: Random Composites, Mesoscale Micromechanics, Statistical Volume Elements, Probabilistic Methods

1 INTRODUCTION

It is often necessary to describe the response of a heterogeneous material in a probabilistic framework so that the uncertainties in local material behavior can be propagated to macroscale behavior. To do so at the microscale may require large computational expense, and material microstructures may be difficult to simulate directly. Instead, if the material can be modeled at the mesoscale, local variability can be retained at no cost to computational efficiency. In this way, material property parameter distributions are generated that can be used as a basis for stochastic simulation.

A challenge arises in characterizing material behavior at the mesoscale, however, since the material properties obtained are typically dependent on the type of loading applied. For example, uniform traction boundary conditions produce a different approximation of effective properties than do uniform displacement boundary conditions; this effect has been well established[1]. A material sample large enough to be characterized independently of loading is referred to as a representative volume element (RVE). The RVE then represents an equivalent homogeneous material with effective properties. A hierarchy of bounds has been established in which the average apparent properties of SVEs that partition an RVE have been shown to decrease with increasing size of the partitions. In particular, a uniform displacement boundary condition approach will produce average apparent properties that bound the RVE effective property from above. The tightness of this bound increases as SVE partition size increases.

It is useful to characterize local material variability, while prioritizing computational efficiency, in order to facilitate probabilistic simulation. In a probabilistic framework, statistics on material variability can help inform stochastic simulations of composite material behavior[2]. To do so, however, the apparent behavior at the material mesoscale must be accurately characterized. Recent work has shown that when partition geometry reflects the underlying material microstructure, material property bounds can be improved[3]. In this work, an approach is presented where polygon cells created by Voronoi tessellation are used to partition the material microstructure into SVEs. These polygons are constructed such that their boundaries do not intersect the inclusions of the material microstructure. The resulting SVE properties are compared with results obtained using square partitions, where partition boundaries often intersect inclusions. Each partitioning method is used to generate a population of apparent properties for a given material. Probability distribution functions are generated from each sample of apparent properties using the Principle of Maximum Entropy[4] (MaxEnt), and used to visualize the impact of different schemes and track the convergence of the material property mean values[5].

In addition to comparing the effect of partitioning scheme (Voronoi or square) on these PDFs, the effect of partition size is also studied. In other works[6] the question determining an optimal length scale for partitioning has been presented as a central question; where partition size is too small, the material property field is too noisy, and where it is too large, useful characterization of local variability is obscured by averaging. Characteristics of the material, including material contrast ratio and morphology, are also varied in this study. Three contrast ratios of inclusion to matrix material are considered (10:1, 100:1, 1000:1). Two material microstructures are considered: one with uniformly randomly distributed circular inclusions, and one with clustered randomly distributed inclusions. This work investigates the effect of the choice of partition scheme and partition size on characterization of materials with different properties and morphology.

2 METHODS OF PARTITIONING

Two square RVEs are constructed containing circular inclusions. The material is determined to behave as an RVE when the side length of the RVE is 100 times the circular inclusion diameter. The inclusion volume fraction of the RVE is 0.10. The RVEs constructed differ in morphology: fig.1a shows the first RVE, which has uniformly randomly distributed circular inclusions, and fig.1b shows the second RVE, which has clustered randomly distributed circular inclusions.

The first microstructure morphology was generated by uniformly placing inclusion center points using a Poisson process. The morphology of the second microstructure was created in two stages. First, center points of inclusion “clusters” were uniformly randomly placed using a Poisson process in a similar manner as for the first RVE. Within these clusters, inclusions were then placed within a given radius of the each cluster center point. The initial spacing of the cluster center points and the area of each cluster region were controlled so that the overall volume fraction of inclusions was approximately the same as in the first microstructure (0.10).

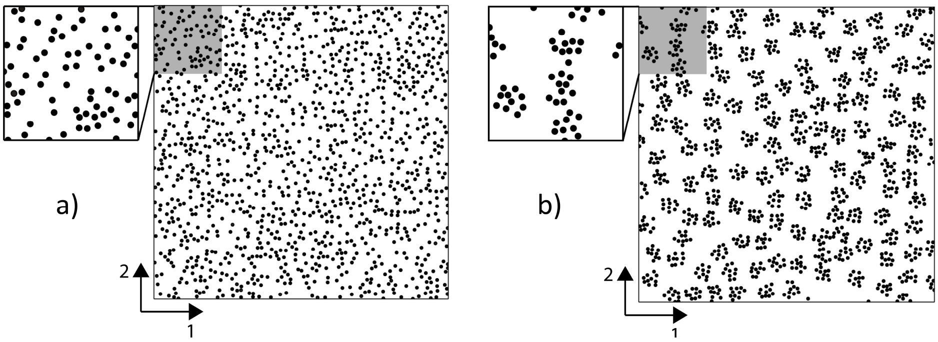

Figure 1: a) Composite microstructure, with uniformly randomly distributed circular inclusions b) Composite microstructure with clustered randomly distributed circular inclusions.

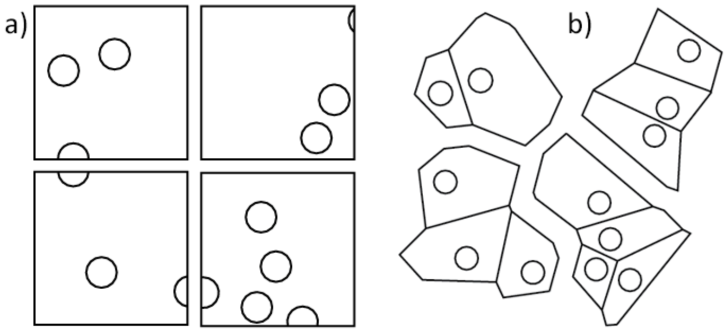

Figure 2: a) Square partitioning at partition scale, $\delta = 5$ b) Similarly sized grouping of cells using Voronoi tessellation partitioning, $\delta = 5$.

These two RVE microstructures (referred to as “uniform” and “clustered”) were then subdivided using two different partitioning schemes. The square partitioning technique, illustrated in fig.2a, evenly divides each RVE into square regions. Since inclusions are randomly placed, partition boundaries often intersect inclusions, as seen in fig.2a.

In the second partitioning scheme, shown in fig.2b, a Voronoi tessellation scheme is used to subdivide each microstructure into a collection of space filling polygon cells. Each polygon is constructed around the center point of an inclusion. The boundaries of each polygon then include all of the material that lies closer to that inclusion than to any other. Voronoi polygon boundaries are constructed so as not to intersect any inclusions. In order to facilitate the comparison with square grid partitioning, the polygons are grouped together, as shown in fig.2b, to generate SVEs whose sizes are approximately the same as the square SVE shown in fig.2a. This is achieved by calculating the centroid of each polygon. If the centroid lies within the area given by the square partition, at a particular grid location, the polygon is assigned to that grouping. In this way, groupings of Voronoi polygons are generated whose total area is similar to the size of each square partition.

Several length scales were used in partitioning. A partition scale, δ is defined as the characteristic size of the SVE divided by the inclusion diameter. Using this definition, the partitioning scales used in this work are $\delta = 5$, 10, and 100. These partition the RVE into SVE populations of 400, 100, and 1, volume elements, respectively. When $\delta = 100$, the RVE is recovered. Each SVE is then evaluated to determine its apparent properties, as described below.

3 EVALUATION OF MATERIAL PROPERTIES

In order to calculate material properties, including the effective properties of each RVE and the apparent properties of each SVE, a finite element analysis was performed on each microstructure. The boundary conditions used were uniform displacement, as these are more appropriate than traction boundary conditions when using FEA[7]. According to the hierarchy of bounds on material effective behavior, these tests produce a set of upper bounds. [1, 8]

To calculate material properties, the strain energy (U) was recovered from the output of FEA for each boundary condition test. When the applied uniform strain (ε^0) is known, the entries of the constitutive tensor (C_{ijkl}) can be calculated by the following equation as given in[8]:

$$
\begin{aligned}
U &= \frac{V}{2}\left[\overline{\sigma}_{ij}\varepsilon_{ij}^{0}\right] \\
&= \frac{V}{2}\varepsilon_{ij}^{0}C_{ijkl}\varepsilon_{ij}^{0} \\
&= \frac{V}{2}\Big[C_{1111}\left(\varepsilon_{11}^{0}\right)^{2} + C_{2222}\left(\varepsilon_{22}^{0}\right)^{2} + C_{3333}\left(\varepsilon_{33}^{0}\right)^{2} \\
&\quad + 2\varepsilon_{11}^{0}C_{1122}\varepsilon_{22}^{0} + 2\varepsilon_{22}^{0}C_{2212}\varepsilon_{12}^{0} + 2\varepsilon_{12}^{0}C_{1211}\varepsilon_{11}^{0}
\end{aligned}
\tag{1}
$$

where V is the volume of the material tested. All material properties can be calculated by this method; in this work, only the axial load test results are presented, generating an approximation of the material property parameter (C_{1111}).

4. RESULTS

Results show the influence of partition size and phase contrast ratio, (E_{fiber}:E_{matrix}) on the distribution of material properties given by square and Voronoi partitioning. Three contrast ratios were investigated: 10:1,100:1 and 1000:1. In each case, the elastic modulus of the fiber was varied, and the elastic modulus of the matrix held at 1 GPa. Three partition sizes were compared, $\delta = 5, 10, 100$, where $\delta = 100$ represents the RVE.

A preliminary study of the effect of varying microstructural morphology is also presented by considering the differences between the uniform and clustered microstructures. The results are visually and statistically contrasted using probability distribution functions (PDFs) of the apparent properties for each case. These PDFs were developed using the Principle of Maximum Entropy (MaxEnt) [4].

Figure 3 shows probability density functions generated using MaxEnt for a material with contrast ratio 10:1, for the three different partition sizes and two partitioning schemes. As expected based on the established hierarchy of bounds, results show a decrease in the mean value of the SVE apparent properties with an increase in partition size. This hierarchy holds for both types of partitioning. However, the mean values based on the Voronoi partitioning scheme are closer to the RVE values, for a given partition size, than those based on square partitioning.

Figures 4 and 5 show results for the case of contrast ratio 100:1 and 1000:1, respectively. The same trends are seen with respect to increasing partition size (closer SVE bounds on the effective property) and with respect to square and Voronoi partitioning.

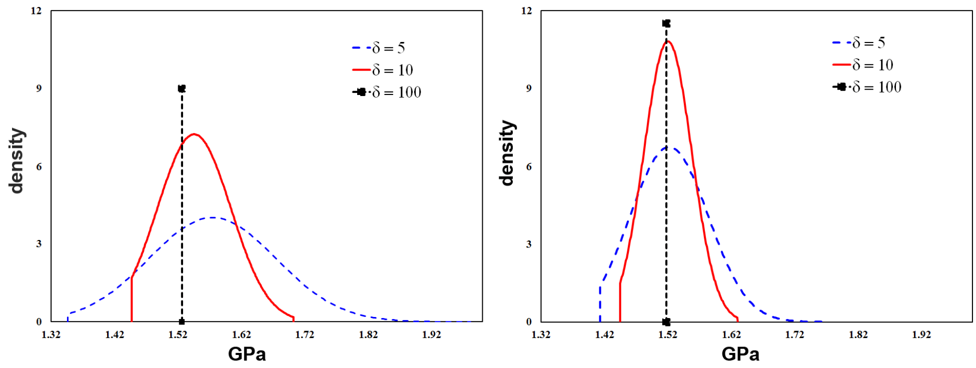

Figure 3: Probability distribution functions for materials with 10:1 contrast ratio. Uniform microstructure with characteristic SVE partition dimensions δ = 5, 10 and 100 is shown. Results are for a) square grid partitioning, and b) partitioning by Voronoi tessellation.

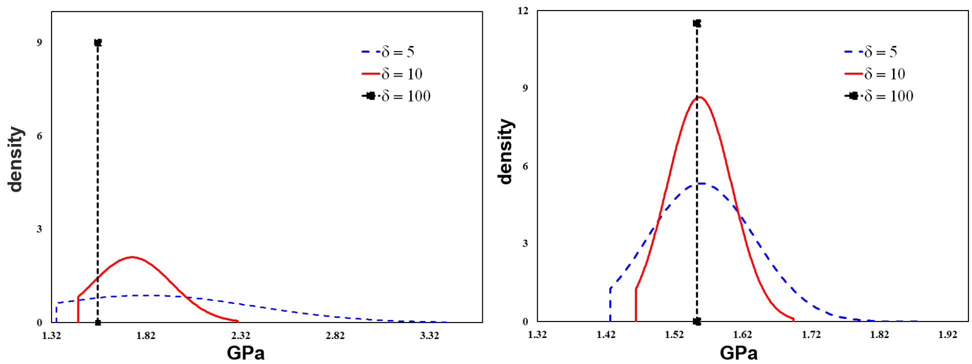

Figure 4: Probability distribution functions for materials with 100:1 contrast ratio. Uniform microstructure with characteristic SVE partition dimensions δ = 5, 10 and 100 is shown. Results are for a) square grid partitioning and b) partitioning by Voronoi tessellation.

When comparing the effect of increasing the material contrast ratio in figs.3-5, the advantage of using a Voronoi partition scheme becomes more evident as the contrast ratio increases. When highly stiff particles intersect the boundary of an SVE partition they have a large effect on the apparent properties of the SVE, shifting the mean value artificially higher. Voronoi partition boundaries avoid this effect.

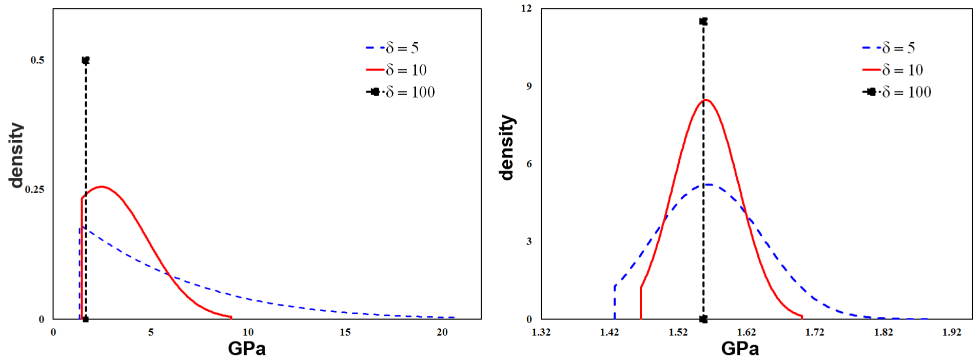

Figure 5: Probability distribution functions for materials with 1000:1 contrast ratio. Uniform microstructure with characteristic SVE partition dimensions δ = 5, 10 and 100 is shown. Results are for a) square grid partitioning and b) partitioning by Voronoi tessellation.

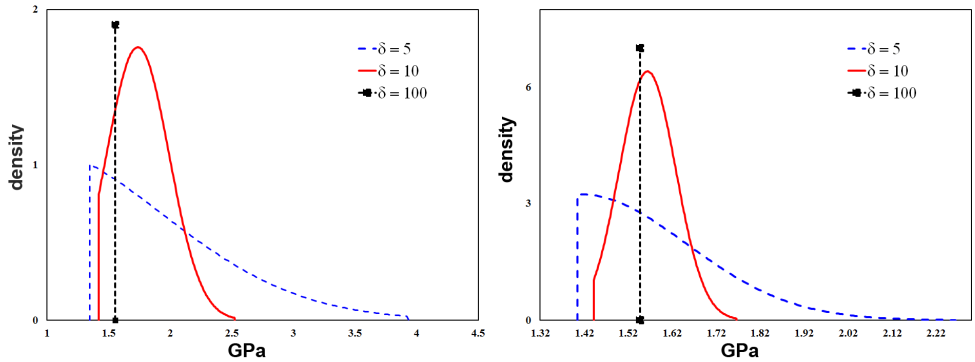

Figure 6: Probability distribution functions for materials with 100:1 contrast ratio. Clustered microstructure with characteristic SVE partition dimensions δ = 5, 10 and 100 is shown. Results are for a) square grid partitioning and b) partitioning by Voronoi tessellation.

Figure 6 shows results for the clustered microstructure, shown in fig.1b. Again, the hierarchy of bounds on the mean of the SVE behavior is evident for both square and Voronoi partitioning. Voronoi partitioning produces SVE distributions closer to the RVE mean value, i.e. lower upper bounds. In the case of the partition size $\delta = 10$ the Voronoi distribution is much more symmetric in appearance than that generated by square partitioning, an effect which is also seen in the uniform case (figs.3-5).

To more directly compare the difference based on microstructure, fig.7 shows zero mean field probability distributions for the clustered and uniform microstructures for a single contrast ratio and partition size (100:1 and 10, respectively). These preliminary results suggest that Voronoi partitioning may more accurately distinguish the effect of microstructural morphology on the probability distribution of material property parameters at the mesoscale.

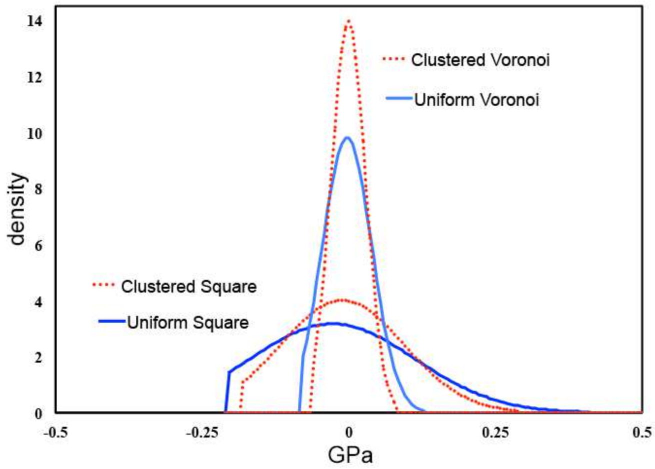

Figure 7: Probability distribution functions based on uniform and clustered microstructures. Zero mean field distributions are shown for comparison. Contrast ratio is 100:1, and characteristic SVE partition dimension is $\delta = 10$. Results are given for square grid partitioning and partitioning by Voronoi tessellation.

5. CONCLUSIONS

Statistical volume elements were generated using two different partitioning schemes (square and Voronoi) with various partition sizes and on two model material microstructures. These model materials varied in phase contrast ratio and microstructural morphology. In each case, apparent properties were determined by the solution of boundary value problems on each SVE. The distributions of these apparent properties were then approximated using the Principal of Maximum Entropy.

The results show a consistent advantage to using a Voronoi scheme to partition the RVE. Voronoi partitioning results are less sensitive to partitioning length scale; Voronoi partitioning produces results at smaller length scales which are more accurate in the sense that the population means more closely matches the RVE mean. Also, Voronoi partition results generate material property PDFs that exhibit less sensitivity to material contrast ratio. Finally, a preliminary investigation comparing the results for microstructures with uniform and clustered microstructures suggests that Voronoi partitioning is more likely to generate material property distributions that capture the effects of the material microstructure.

Each of these advantages of Voronoi partitioning is potentially important in the use of mesoscale material property distributions as a basis for stochastic simulation. This work may ultimately inform the study of material reliability, by characterizing probabilistic behavior of materials that leads to uncertainty in material response.

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