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An efficient Method to Reconstruct Random Heterogeneous Material Properties

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ABSTRACT

At the present time, understanding and controlling the microstructure of the materials is of great technological importance. In fact, the properties of a material as a whole are, in general, determined not only by the physical/mechanical features of the microscopic constituents, but also by their geometry and distribution. The presence of uncertainties/perturbations in experimental studies or the intrinsic uncertainties in the microstructure of the materials implies that these input parameters have some inherent uncertainties and therefore they can be characterized only statistically. To accurately predict the performance of the random materials, it becomes essential to include the effects of these uncertainties into the simulation model and understand how they propagate and alter the final solution (i.e. the macroscopic quantities of interest).

Recently, methods based on pattern recognition and classification techniques have been used in analysis and design problems of materials (see e.g. [2, 5, 4]). These approaches provide relationships between the microstructure descriptors and the macroscopic behavior of the materials. These methods may prove to be particularly useful within the context of large scale computational approaches by providing a tool to identify the critical microscopic configurations. However, the study of the material behavior in non-trivial cases can be only obtained adopting numerical tools that inevitably create demands for efficient computational strategies and algorithms to generate and analyze the samples of the microstructure of the random materials. These approaches allow to avoid or limit the testing of real materials which are more expensive or even impractical than the numerical analysis.

The reconstruction process of the microstructure starts from statistical information obtained experimentally (e.g. X-ray microscopy, Transmission Electron Microscopy [1, 6]) or from hypothetical models. Stochastic optimization algorithms have been already successfully applied to the reconstruction of multiphase microstructures of Random Heterogeneous Media [3]. However, the classification techniques require a large data set and not only a single or few realizations of the microstructure. Moreover the reconstructed microstructure is not unique since usually only a limited amount of information of the underlying process is provided.

In this work an efficient approach to generate a database of microstructures is proposed. A hybrid method based on the synergy between Genetic Algorithms (GA), Simulated Annealing (SA) and Tabu

list is suggested. In particular, the GAs are adopted to efficiently identify the microstructure configurations that satisfy the selected descriptors of the material. The SA technique is adopted to refine the solutions identified by the GA. A Tabu list, based on a sort of measure of the "distance" between the microstructure samples, is adopted to generate a database that contains only the most significant microstructure configurations avoiding the presence of equivalent or duplicate microstructures.

In summary, a very efficient procedure to generate samples of the microstructure of random heterogeneous media starting from limited amount of information is presented. The subsequent analysis (i.e. FEM analysis) can be performed to obtain the desired macroscopic properties providing a link between the micro- and the macro-scale.

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