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Microstructure Informatics Using Higher-Order Statistics and Efficient Data-Mining Protocols

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Summary

Microstructure Informatics is a critical building block of ICME infrastructure. Accelerated design and development of new advanced materials with improved performance characteristics and their successful insertion in engineering practice are largely hindered by the lack of a rigorous mathematical framework for the robust generation of microstructure informatics relevant to the specific application. In this paper, we describe a set of novel and efficient computational protocols that are capable of accelerating significantly the process of building the needed microstructure informatics for a targeted application. These novel protocols have several advantages over the current practice in the field: (i) they allow archival, real-time searches, and quantitative comparisons of different instantiations within large microstructure datasets, (ii) they allow for automatic identification and extraction of microstructure features or metrics of interest from very large datasets, (iii) they allow for establishment of reliable microstructure-property correlations using objective measures of microstructure, and (iv) they provide precise quantitative insights on how the local neighborhood influences the localization of macroscale loading and/or the local evolution of microstructure leading to development of robust, scale-bridging, microstructure-property-processing linkages.