## **Defense Announcement**

Computational modeling of wave propagation in heterogeneous microstructures using discrete and continuum frameworks

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With the recent advances in material science and additive manufacturing, there has been an ever-growing trend in developing materials with novel properties. These materials are often heterogeneous composites—with complex microstructures influencing their overall structural behavior. Though non-destructive evaluation using wave propagation can offer the mechanical properties of the composite, experimental methods to gain insights into the relationship between microstructure and mechanical properties can be cumbersome and time-consuming. Hence, researchers prefer computational modeling of materials to trial-and-error experiments.

Among the contemporary numerical methods to study heterogeneous materials, discrete lattice models can seamlessly incorporate complex microstructural heterogeneities into the model. However, the available lattice models suffer from numerous deficiencies such as the limitation of Poisson's ratio, not being isotropic (naive square lattice), incorporating additional elements or additional degrees of freedom, and not practical for complex domains (equilateral triangle, hexagon lattices). Hence, we aim to develop a lattice model that can span the admissible Poisson's ratio values with a minimum number of elements and degrees of freedom. We use the Lagrangians in continuum and discrete systems, identify the shortcomings in the lattice model and offer a solution to make the lattice isotropic without the limitation of Poisson's ratio. This model is verified on the benchmark problems and applied to study wave propagation in the heterogeneous microstructure of hydrated cement paste.

Furthermore, studying the influence of microstructure on wave propagation in heterogeneous materials needs exploring different material classes with distinct mechanical properties. Given the number of input parameters to operate with, one needs sensitivity analysis to reduce the dimensionality of the input parameter space. One among the many available techniques is the Shapley value—a solution concept from cooperative game theory to identify the marginal contribution of the individual parameters—was recently being used in machine learning to quantify the weights of a neural network. In this work, this technique is applied to rank the input parameters based on their influence on wave attenuation in materials with matrix-inclusion morphology of circular inclusions.