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MULTISCALE MODELING OF RANDOM LATTICES: CRITICAL ISSUES ON CONTINUUM APPROXIMATION

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ABSTRACT

In this work, we are concerned that transmission of various boundary conditions through irregular lattices. The boundary conditions are parameterized using trigonometric Fourier series, and it is shown that, under certain conditions, transmission through irregular lattices can be well approximated by that through classical continuum. It is determined that such transmission must involve the wavelength of at least 12 lattice spacings; for smaller wavelength classical continuum approximations become increasingly inaccurate.

PROBLEM FORMULATION

For many problems associated with fracture and microscopic pattern formation, the primary objective is to compute microscopic quantities relevant to the phenomenon of interest. Accordingly, we focus not on the continuum model but on how its introduction affects the microscopic quantities of interest. Furthermore, in contrast to the majority of multiscale models involving continuum components, we engage the continuum model not as a component of a multiscale model, but rather as a generator of a limited approximation basis for exact solutions of boundary-value problems defined for the exact lattice model.

Consider a two-dimensional irregular lattice constructed according to the following procedure: (i) the nodes are generated as a set of points whose cartesian coordinates are uniformly distributed random variables, and (ii) the nodes are connected by the bonds following the Delaunay triangulation. We refer to such lattices as Delaunay random lattices. We assume that the lattice is subjected to anti-plane deformation and its bonds exhibit linear elastic behavior characterized by the stiffness inversely proportional to the bond length. This dependence is consistent with the assumption that all bonds have the same shear modulus and in-plane thickness.

For very large lattices, one needs to develop a multiscale representation that delivers accurate predictions for the quantities of interest using significantly reduced amounts of data and arithmetic operations. Let us consider a circular lattice Ω of radius R. The lattice is subjected to prescribed displacements at the exterior nodes $\partial\Omega$, while the rest of the nodes are unloaded; we denote the vector of prescribed displacements by ϕ. We define the domain of interest ω as a circle of radius r ($r < R$) concentric with Ω. We define as the quantities of interest the nodal displacements of $\partial\omega$ and denote them by ψ. By restricting the quantities of interest to the boundary, we suppose that all other nodal displacements of ω are less prone to errors associated with multiscale representation. The matrix relating the input ϕ to the output ψ is referred to as the transmission matrix:

$$\psi = T\phi\,.$$

This dimensionless matrix T is uniquely defined by the lattice geometry.

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Following the structure of multiscale models involving discrete and continuum components [1], we partition Ω into three concentric domains: (i) domain of interest ω (circle of radius r); (ii) deterministic buffer zone (ring with radii r and $\rho = r + \delta$); (iii) statistical buffer zone (ring with radii ρ and R). In simulations, at first, the entire lattice is generated as a Delaunay random lattice. Then, the nodes inside the domain of interest and deterministic buffer zone are retained, whereas the nodes inside the statistical buffer zone are generated anew. The adopted structure of the statistical buffer zone is consistent with the view that the continuum model can be derived via ensemble averaging. Also, it is appropriate to treat the transmission matrix as a random variable, and focus on computing its mean value $\bar{T}$ via ensemble averaging.

The singular value decomposition theorem is a natural way of evaluating the transmission matrix:

$$\bar{T}_{m\times n} = U_{m\times m} S_{m\times n} V^{*}_{n\times n}\,.$$

Here the asterisk denotes matrix transposition. The matrix dimensions $m \times n$ represent the number of nodes of $\partial\omega$ and $\partial\Omega$, respectively; of course $m < n$. For a detailed description, the reader may refer to [2].

The singular value decomposition theorem lends itself to a transparent and useful interpretation, once we regard ϕ as an input and ψ as the corresponding output. Then the vector $V^*\phi$ represents the input as a superposition of n orthogonal inputs. The structure of the matrix S implies that out of n of those inputs only the first m are transmitted; the singular values represent the weights assigned to those m inputs. Finally, the matrix U converts the m weighted orthogonal inputs into the output column-vector ψ of size m. A meaningful comparison of $\bar{T}$ with its counterpart based on a continuum model must be restricted to comparisons of the matrices S and V, as they control how the input is structured. In contrast, the matrix U controls how the input is converted into the output in the domain of interest. Details of that conversion are significantly affected by the local microstructural details and therefore cannot by captured by the continuum model. The spectral structure of the V-matrix for a circular lattice is trigonometric, which implies that the processed input $\mathbf{V}^*\phi$ is a superposition of waves generated by the mode functions $\cos(k\theta)$ and $\sin(k\theta)$. Accordingly, one should expect that the continuum model may be useful only for $k < k_0$, where k_0 is a threshold wave number that depends on tolerance ε and possibly other problem parameters.

Simulation Results

The characteristic lattice spacing is defined as 1 in simulations by specifying the areal node density μ. In Figure 1, we show two modes of V-matrix corresponding to $\rho = 25$, $\delta = 5$, and $\Delta = 20$. There the continuous lines and discrete symbols represent the exact and approximate solutions, respectively. The quality of approximate solutions deteriorates for high order modes. The threshold wavelength should be a lattice property, which is defined as

$$\lambda_0 = \frac{\pi\rho}{i_0}\,.$$

The relationship between mode number i_0 and wave number k_0 is described in [2]. Further simulation results support a constant $\lambda_0 \approx 13$ may be used as a uniquely defined threshold for a specific tolerance $\varepsilon = 0.3$. We repeated the entire study for S. This did not change the overall trend but led to a slightly lower threshold $\lambda_0 \approx 12$. The size effects of ρ, δ, and Δ cannot be discussed here for lack of space, but the interested readers may refer to [2] for details.

CONCLUSIONS

In this paper, we defined a restricted class of continuum models and determined conditions under which solutions of such models are sufficiently close to the exact solutions. It is shown that, the continuum approximations are accurate for the wavelength of at least 12 lattice spacings. Our views echo results obtained by Babuska and co-workers on the penetration function [3].

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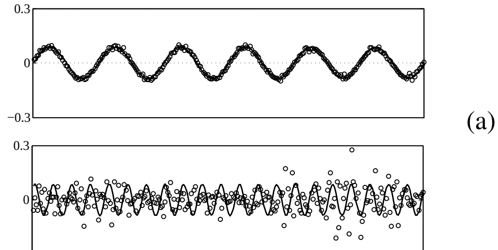

FIGURE 1. Discrete (symbols) versus continuum (lines) modes for $\rho = 25, \delta = 5, \Delta = 20$: (a)mode number 12, (b) mode number 42.

