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Shape Design Sensitivity Analysis of Nanoscale Lattice Structures

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Due to the rapid development of nanotechnologies, the necessity of nanoscale analysis in both analysis and design problems is continuously increasing. Molecular dynamic (MD) simulation which is a typical transient dynamic problem is utilized in various applications such as dislocation, crack propagation, and strain localization since these include the microscopic behavior which cannot be captured in continuum sense. Also the nanoscale material properties are investigated by using MD simulation. Much research effort is concentrated on the size or shape effects of the mechanical properties such as Young's modulus and yield stress for the nano wires and nano particles. In the viewpoint of design, it is inevitable to develop shape design sensitivity analysis method considering such nano scale shape effects.

Generalized Langevin equation (GLE) is derived by Adelman and Doll [1, 2] to eliminate the unnecessary atomic DOFs to analyze atomic motion in a locally confined region of interest. The effects of the eliminated atoms are treated at the boundary as a damping force consisting of a damping kernel matrix and the velocity of atoms. The reduced atomic system can be constructed to avoid the huge computational costs for the full MD considering the effects of surrounding utilizing generalized Langevin equations.

In this research, we presented the shape design sensitivity analysis (DSA) method for nanoscale lattice structures using generalized Langevin equation. The conventional shape design sensitivity analysis method based on material derivative concept cannot be applied to the molecular dynamic system since the performance measure is not a continuous function with respect to the shape design variables. Therefore, discrete shape variation is transformed into GLE impedance forces so that the shape design sensitivity analysis problem is successfully converted to a non-shape problem. The effects of the added atoms as a result of shape perturbation are treated as GLE impedance forces on the interface between original and perturbed shapes. Through some numerical examples, the derived shape design sensitivities based on GLE turns out to be accurate compared with finite differences. Especially for the crack propagation problem, the direction of crack propagation can be predicted from a what-if study utilizing the derived shape sensitivities for the cento-symmetry parameters [3].

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