Continuum-based Shape Sensitivity Analysis for 2-D Coupled Atomistic/Continuum Simulations Using Bridging Scale Decomposition

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Abstract

In this paper we present a continuum-based shape sensitivity analysis for two-dimensional coupled atomistic and continuum problems using bridging scale decomposition. The bridging scale method is one of the most advanced multi-scale simulation methods developed recently. It provides a simplified treatment of the interface between atomistic and continuum simulations. The proposed sensitivity analysis approach is developed based on a continuum variational formulation of the bridging scale. The sensitivity expressions for both direct differentiation method (DDM) and adjoint variable method (AVM) are derived in a continuum setting by taking material derivative of the continuum energy equations directly before discretization, rather than differentiating discrete bridging scale differential equations. This continuum sensitivity formulation provides a versatile and unified system of equations in representing the nature of multi-scale structural problems, and is in general more desirable than that of the discrete approaches. Due to its computational advantage for crack propagation problems, the direct differentiation method is chosen to be implemented numerically and has been applied to two examples, including a two-dimensional crack propagation problem. To overcome the issue of discontinuity in shape design due to the discrete nature of the molecular dynamics (MD) simulation, we define design velocity fields in a way that the shape of the MD region does not change with design. This can be justified by the fact that the MD region is in general much smaller compared with the entire structural domain, and that design velocity fields can always be chosen arbitrarily as long as the velocity fields satisfy the continuity and regularity requirements. In addition, since the discrete FE mass matrix in bridging scale is not continuous with respect to shape design variables, we assume an evenly distributed mass density when evaluating the material derivative of the FE mass matrix. It is demonstrated in our numerical examples that even with this approximation, desirable sensitivity accuracy can be achieved as long as the number of atoms per element is sufficiently large. In order to support design perturbation of the FE mass matrix in bridging scale, we use regular-shaped finite elements and only allow shape change in one direction in our example problems. However, the sensitivity formulation derived is sufficiently general to support irregular-shaped finite elements and arbitrary design velocity fields for two-dimensional structures. The sensitivity results, which are verified by using overall finite difference method, reveal the impact of macroscopic shape design change on microscopic crack propagation, which can be explained with basic physics.

Keywords: *bridging scale method, multi-scale simulation, shape sensitivity analysis.*

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