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# MULTISCALE ADJOINT DESIGN SENSITIVITY ANALYSIS OF TRANSIENT DYNAMICS

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## Abstract

A multiscale adjoint design sensitivity analysis (DSA) for transient dynamics is developed using orthogonal scale decomposition. For efficient DSA, bridging scale method (BSM) is utilized as a response analysis and the adjoint variable method (AVM) is applied in sensitivity analysis. By using mass weighted projection operator not only for original responses but also for adjoint variables, a fully decoupled equation of each scale is derived for sensitivity analysis as well as for the original response analysis and we were able to avoid any iterative computations between the scales.

Recently, MD simulation is often utilized in various applications such as dislocation, crack propagation, and strain localization, which cannot be captured by continuum sense. However, multiscale DSA is not a straightforward method since the sensitivity relations between the scales are not well known. Even if the relations are known, iterative sensitivity computations might be needed if the scales are coupled. Furthermore, the finite difference method (FDM) is not applicable for such transient dynamics, which have highly nonlinear design variables, since the accuracy of the design sensitivity is not guaranteed due to the dependency on the amount of perturbation.

The purpose of this research is to develop efficient and accurate multiscale DSA for transient dynamics. In BSM, the total displacement is decomposed into fine and coarse scales by the projection of MD solution onto the coarse scale. The projection operator is obtained by the minimum condition of mass weighted error measure between the MD and finite element (FE) solutions. This type of projection operator enables us to derive fully decoupled multiscale equations of motion for each scale. Furthermore, through generalized Langevin equation (GLE), MD simulation is considered only for locally confined region instead of the entire domain. In addition, FE analysis for the coarse scale solution is performed on the whole region to obtain global performance. In DSA, we use the bridging scale decomposition not only for total displacement but also for the total adjoint response to derive multiscale adjoint equations. By applying GLE force in the fine scale adjoint equation, a bridging scale adjoint equation is derived which is the adjoint system of the multiscale bridging scale equations. This enables us to perform the fine scale DSA for a local confined region. Therefore, the efficiency of DSA is obtained by fully decoupling the adjoint response, and by reducing the MD region imposed with GLE force. Time integration is only once more needed for the bridging scale adjoint equations regardless of the number of design variables compared to other methods such as the direct differential method (DDM) and FDM.

Through numerical examples of the crack propagation problem, the accuracy and efficiency of developed bridging scale DSA is verified compared with finite difference sensitivity.

**KEY WORDS**: Multiscale transient dynamics design sensitivity analysis, Bridging scale adjoint design sensitivity, Adjoint variable method (AVM), Bridging scale method (BSM), Generalized Langevin equation (GLE)