Adjoint Design Sensitivity Analysis of Atomistic Structures based on Generalized Langevin Equation

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Due to the limitation of computing power, adjoint design sensitivity analysis (DSA) in molecular dynamic (MD) simulations is nearly impractical in efficiency and accuracy. However, a generalized Langevin equation (GLE) could reduce the full MD domain to a locally confined region, considering the effects of surrounding. We present an efficient DSA method for periodic lattice structures where a reduced atomic system is constructed in a locally confined region. The effects of eliminated atoms are treated at the boundary as a damping force consisting of a damping kernel matrix and the velocity of atoms. Due to the translational symmetry in lattice structures, the size of time history kernel function that accounts for the boundary effects of the reduced systems could be reduced to a single atom's degrees of freedom. Through numerical examples, the developed analytical DSA method turns out to be accurate and efficient in comparison with finite differencing.

Keywords: Adjoint design sensitivity analysis, Molecular dynamic (MD) simulation, Periodic lattice structures, Generalized Langevin equation (GLE), Time history kernel

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