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Efficient coarse-graining of boundary surface for solving Atomistic/Continuum multiscale problems using Green's function

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An atomistic discrete counterpart to the Boundary Element Method uses a Lattice Green's Function Method (LGFM) to efficiently solve three-dimensional Atomistic/Continuum multiscale boundary value problems [1]. In practical boundary value problems, the boundary surface may contain millions of degrees of freedom due to the atomistic resolution. Since the forces and displacements on the boundary at the atomic scale are expected to be slowly varying, a coarse-graining method is introduced here. We interpolate boundary displacements/surface forces using boundary shape functions [2] and highlight the importance of special treatment of edges and corners due to the LGFM formulation. Further, we introduce hierarchical matrices [3] to approximate the dense coarse-grained Green's function matrices as a means to reduce memory and computation time during the simulations. The interplay between the different numerical length scales introduced via both coarsening and hierarchical matrix approximation is evaluated in terms of memory, computation time, and accuracy, using simple boundary value problems.

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