Parallel Multi-Scale Computation Using the Message Passing Interface

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Abstract

A sequential three-dimensional hybrid molecular dynamics (MD)/finite-element (FE) code to perform continuum and atomistic multi-scale modeling and computation, has been parallelized using the Message Passing Interface (MPI) library. A master-slave divide-and-conquer approach, emphasizing the functionality and robustness of the code, is implemented through loop parallelism and has reduced execution time: yielding a speedup of greater than 3 and has shown potential for further speedup. The smoothness of the stress distribution across the overlapping region between the continuum domain and the atomistic domain demonstrates the suitability of this method to nanostructure modeling.