Abstract

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Project Title: Development of a Fast, Scalable Reactive Molecular Dynamic Simulation Program Using Dynamic Bond-Order Potentials on Many-Integrated Core Computation Platform

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Abstract:

Molecular dynamics (MD) simulation is an important tool for numerous research areas. However, MD simulation encompasses large spatio-temporal scale is required to characterize real-world system. Lack of fast and scalable reactive MD simulation program for modern computer platforms limit a capability to solve practical problem. In this work, we have developed a new and efficient reactive many-body MD program (SCoReMD) based on novel and efficient dynamic *n*-tuple computation. Performance excellence of SCoReMD is achieved through two-tier optimization: (1) Algorithmic-tier via the novel shift/collapse (SC) algorithm on neighbor-list data structure; and (2) Architecture-tier via platform-specific optimization using novel hybrid message-passing and multithreading parallelization technique for multicore and many-integrated core (MIC) computer platforms. Our benchmark results indicated that new neighbor-list based SC-algorithm speedup computation time by 1.33× up to 3.29× for MD simulation with 24 and 24,000 atoms per compute core, respectively. Platform-specific optimization using hybrid MPI/OpenMP/MIC parallelization scheme showed runtime speedup up to 3.06×. The remarkable performance speedup from SCoReMD is expected to significantly improve reactive atomistic simulation time-to-solution, allowing large-size and long-time scale theoretical studies to be performed using modest emerging heterogeneous computer platforms.

Keywords: Parallel algorithm, performance optimization, reactive molecular dynamics, heterogeneous computing, MIC