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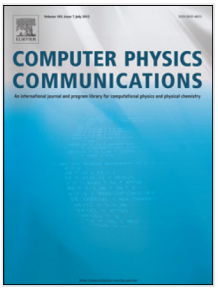

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A hybrid optimization strategy for the communication of large-scale Kinetic Monte Carlo simulation

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Abstract

The parallel Kinetic Monte Carlo (KMC) algorithm based on domain decomposition has been widely used in large-scale physical simulations. However, the communication overhead of the parallel KMC algorithm is critical, and severely degrades the overall performance and scalability. In this paper, we present a hybrid optimization strategy to reduce the communication overhead for the parallel KMC simulations. We first propose a communication aggregation algorithm to reduce the total number of messages and eliminate the communication redundancy. Then, we utilize the shared memory to reduce the memory copy overhead of the intra-node communication. Finally, we optimize the communication scheduling using the neighborhood collective operations. We demonstrate the scalability and high performance of our hybrid optimization strategy by both theoretical and experimental analysis. Results show that the optimized KMC algorithm exhibits better performance and scalability than the well-known open-source library − SPPARKS. On 32-node Xeon E5-2680 cluster (total 640 cores), the optimized algorithm reduces the communication time by 24.8% compared with SPPARKS.

Keywords:

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