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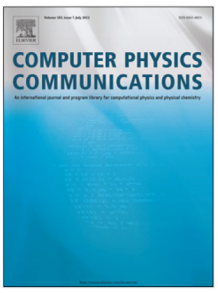

A hybrid algorithm for parallel molecular dynamics simulations

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A hybrid algorithm for parallel molecular dynamics simulations

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Abstract

This article describes algorithms for the hybrid parallelization and SIMD vectorization of molecular dynamics simulations with short-range forces. The parallelization method combines domain decomposition with a thread-based parallelization approach. The goal of the work is to enable efficient simulations of very large (tens of millions of atoms) and inhomogeneous systems on many-core processors with hundreds or thousands of cores and SIMD units with large vector sizes. In order to test the efficiency of the method, simulations of a variety of configurations with up to 74 million atoms have been performed. Results are shown that were obtained on multi-core systems with Sandy Bridge and Haswell processors as well as systems with Xeon Phi many-core processors.

Keywords: molecular dynamics, hybrid parallelization, SIMD, Xeon Phi
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1. Introduction

Molecular dynamics is an important tool for the computational modelling of materials. On high-performance computers, large-scale molecular dynamics

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