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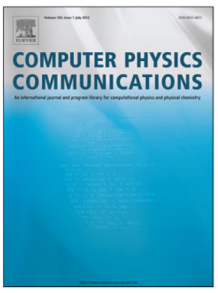

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Suppressing correlations in massively parallel simulations of lattice models

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Abstract

For lattice Monte Carlo simulations parallelization is crucial to make studies of large systems and long simulation time feasible, while sequential simulations remain the gold-standard for correlation-free dynamics. Here, various domain decomposition schemes are compared, concluding with one which delivers virtually correlation-free simulations on GPUs. Extensive simulations of the octahedron model for $2+1$ dimensional Kardar–Parisi–Zhang surface growth, which is very sensitive to correlation in the site-selection dynamics, were performed to show self-consistency of the parallel runs and agreement with the sequential algorithm. We present a GPU implementation providing a speedup of about 30× over a parallel CPU implementation on a single socket and at least 180× with respect to the sequential reference.

1. Introduction

Lattice Monte Carlo (MC) simulations are employed widely to out-of-equilibrium problems [1]. Examples range from growth processes, such as non-equilibrium surface growth [2] or domain growth after phase separation [3], to evolutionary game theory [4]. Simulations of such processes must reproduce the physical kinetics in real systems. This is fundamentally different from equilibrium problems, where it is admissible to change the kinetics to speed up the relaxation, for example by cluster algorithms [5, 6]. Out-of-equilibrium simulations are not at liberty to apply such optimizations.

In practice, the most efficient way to perform lattice MC simulations on a bipartite lattice are checkerboard, or sub-lattice parallel [7], updates, which fit the definition of a stochastic cellular automaton (SCA) [8] since the dynamics considers each site as strictly independent from all other sites on the same sub-lattice. Algorithms of this type can be parallelized very efficiently on many architectures, including GPUs [9–12]. However, in this scheme, the selection of lattice sites is correlated, which influences the kinetics [7]. As we have shown recently [13], this artificial dynamics can indeed affect the dynamical universality class of lattice gas models.

Markov chain MC models, like the Metropolis algorithm [14] and surface growth models [15–18], are usually defined as a series of single-particle updates. To leave the update attempts uncorrelated they must be performed in a random-sequential (RS) fashion, which cannot be parallelized by definition. As an approximation domain decomposition (DD) can be used, where random site selection is restricted to a local domain per parallel worker [19, 20].

Here we review different DD schemes for parallel GPU viable for implementations of lattice MC and present one which is virtually free of correlations. For this purpose we consider the $2+1$–dimensional octahedron model [18] for Kardar–Parisi–Zhang (KPZ) surface growth [21] with RS dynamics and compare autocorrelations for the various types of DD.

In section 2 we define the octahedron model and introduce the basics of KPZ surface growth and aging. The section concludes with a brief summary of properties of the GPU architecture most relevant to this work. In section 3, the considered DD schemes are introduced, their impact on simulation results is presented in section 4, which ends with a comparison of the performance achieved by our implementations. We conclude in section 5.

2. Models and methods

2.1. Octahedron model for ballistic deposition

The octahedron model is illustrated in Fig. 1: Octahedra are deposited or removed at eligible sites with probabilities p and q, respectively. The slopes of the octahedra edges are mapped to a lattice gas with the Kawasaki [22] update rules

$$\begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} \underset{q}{\overset{p}{\rightleftharpoons}} \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix} \quad , \tag{1}$$

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