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Lattice Free Stochastic Dynamics

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Abstract. We introduce a lattice-free hard sphere exclusion stochastic process. The resulting stochastic rates are distance based instead of cell based. The corresponding Markov chain build for this many particle system is updated using an adaptation of the kinetic Monte Carlo method. It becomes quickly apparent that due to the lattice-free environment, and because of that alone, the dynamics behave differently than those in the lattice-based environment. This difference becomes increasingly larger with respect to particle densities/temperatures. The well-known packing problem and its solution (Palasti conjecture) seem to validate the resulting lattice-free dynamics.

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Key words: Lattice-free, microscopic stochastic dynamics, kinetic Monte Carlo.

1 Introduction

Stimulated by the exponential growth in CPU power computationally intensive models and applications have thrived in recent decades. Among them lattice models through Cellular Automaton (CA) and/or Monte Carlo methods have proliferated significantly and are increasingly used to describe and understand a wide variety of complex physical and biological systems [25]. CA for instance have been used in modeling gas phenomena, urban development, immunological processes, and crystallization. The best known application for CA is modeling living systems [26].

Lattice models in conjunction with Monte Carlo methods are often [15] used as a way of modeling systems involving many interacting particles under the influence of noise. Such approaches have been followed in many fields although they are particularly responsible for significant innovation in space and oil exploration [6]. Similarly, molecular dynamics modeling through lattice gas CA or lattice Boltzmann methods are responsible

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for producing a better understanding for a number of fundamental scientific problems in the physics of fluids.

A lattice based model describes a particle system by introducing a spatial discrete lattice consisting of predetermined number of cells within which the particle interactions and dynamics will evolve. One common approach is to built a Markov Chain which evolves the dynamics responsible for constructing the solution of the system. The stochastic dynamics applied depend on the physical properties describing the microscopic interactions for the system. As a result, Metropolis, Arrhenius, Glauber, Kawasaki and other rates are carefully considered depending on the knowledge of the microscopic behavior of the system. The applications of such methodologies range from granular material [14, 19], traffic flow [22], ecology [5, 7], lattice Boltzmann and lattice gas [23, 27], surface growth [13] just to name a few.

In this work we construct a lattice-free (LF) stochastic process. The underlying stochastic dynamics are stripped of their dependence on the usual lattice-based (LB) environment. Interacting particles therefore will be free to land and interact at locations prescribed by the dynamics from stochastic rates which are distance based instead of cell based. For this exposition we equip our stochastic process with an Arrhenius spin-flip (non-conservative), hard sphere, exclusion potential and examine/compare the particle behavior at equilibrium as well as on the transition path to equilibrium. Other potentials can also be considered as well since the findings of this work are not tied to the particular form of the interaction potential used. We furthermore propose a corresponding version of the well-known kinetic Monte Carlo (KMC) algorithm in order to practically implement this LF stochastic process. Although we restrict our exposition in this article to updates performed by the KMC algorithm other updating mechanisms can also be considered and applied in a similar fashion.

We motive the application of LF dynamics by exposing obvious shortcomings in solutions produced by LB dynamics under certain regimes where particle sizes can influence or interfere with their interactions. Under such regimes LB dynamics and corresponding LB models can produce erroneous results with non-physical solutions. This phenomenon occurs for all interaction potentials. The differences in solutions however are most pronounced for model parameters promoting high particle densities. Furthermore, we show that convergence will not fix this discrepancy. In other words, as the lattice size increases the solutions from LB dynamics will not converge to that of the LF dynamics. Clearly the reason for the difference in solutions between LB and LF dynamics simply results from the fact that a lattice, with predefined cells for particles to land in, offers a more efficient use of space. As a result the corresponding density of those particles can be much higher in the case of LB models. Many natural processes involve interactants which move in continuum space and not in preset distances/cells as is the case for LB environments. Thus in several modeling situations such a LB methodology, although easier to implement, will produce wrong solutions.