

# Lattice Molecular Automaton (LMA): A physico-chemical simulation system for constructive molecular dynamics.

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## Abstract

Molecular self-assembly is frequently encountered in biochemical systems generating higher order structures with well defined functionalities. However, the driving forces underlying these processes are not well understood.

The *Lattice Molecular Automaton* (LMA) is a computational tool suitable for simulation of self-organization processes in large scale, molecular systems. This paper introduces the basic computational concepts needed to formulate molecular dynamics and self-assembly in a discrete field, cellular automaton environment: Molecular objects are encoded as data structures on a hexagonal lattice. Propagating force particles together with kinetic and potential energy terms define simulation objects with a minimum complexity (number of physical variables together with interaction functions) with respect to specified molecular dynamics and force field properties. In this paper we focus on the mathematical and algorithmic formulation of a variety of intermolecular interactions through a decomposition of molecular type-specific force fields into discrete fields constructed by propagating force information particles.

As an example, the simulation of polymer dynamics in an aqueous environment is shown. The straight forward implementability of the LMA concept on massively parallel architectures as well as possible applications in the field of Computational Nanotechnology are briefly discussed. Thermodynamical properties together with a variety of other physico-chemical properties of the LMA are discussed in detail in reference [1].

# 1 Introduction

## 1.1 Emergence of Hierarchical Structures in Biochemical Systems

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The formation of hierarchically organized structures seems to be a fundamental property of biochemical systems - and in general macromolecular ensembles exhibiting well-defined functionalities. An extensively studied example of molecular self-assembly is vesicle and membrane formation [2, 3], both composed of amphiphilic polymers solvated in the biological solvent water. The basic question to ask about this and other processes is: What are the driving forces for the formation of such highly ordered structures - and what is the underlying chemical information *exactly* necessary for their dynamic construction?

Whereas the elements of a conceptual framework as well as some of the formal dynamical properties for the emergence of higher order structures in formal systems was described recently [4, 5, 6], the physico-chemical background for the generation of such dynamic phenomena in molecular systems is barely treated.

Experimental work shows a sensitive dependence of the morphology of supramolecular structures as e.g. vesicles on the chemical properties of the underlying lipid molecules [7, 8], but the cause for this sensitivity on the molecular scale (i.e. the microdynamics of the single molecules) remains unclear.

In a theoretical context the notion of critical object complexity [4, 5] becomes important. The critical object complexity defines the least amount of information that needs to be encoded on an object sufficient for the generation of particular, specified higher order structures or other emergent properties generated by the dynamics. In the case of molecular systems, the minimum object complexity defines the amount of chemical information at the molecular (object) level that is necessary and sufficient so that the molecular system is able to generate certain observables. This is achieved by encoding only the relevant interactions between the molecules and their environment (i.e. other molecules of various types). Intrinsic features of e.g. amphiphilic molecules is the hydrophobic tail and a hydrophilic head. Such properties, or the concomitant interaction rules with other molecules as the formation of hydrogen bonds, have to be encoded in the molecular objects. In the common molecular dynamics simulation approaches based on Newton's equations of motion [9], these interactions are modeled

The LMA molecular dynamics is defined by two reservoirs of energy, the kinetic and the potential energy. The kinetic energy is formally driving the molecular system into low energy configurations on the potential energy hypersurface. Kinetic energies are distributed over the (in the case of a hexagonal lattice three) degrees of freedom, following e.g. a Boltzmann distribution, and are distributed to other molecular objects in a collision process applying a hard sphere model. Each molecule has an excluded volume and pairwise collisions conserve momentum in a strict sense. Higher order free molecular collisions and collisions involving polymers do not conserve momentum in a strict manner.

The LMA molecular dynamics is formally implemented in a cellular automaton simulation environment, discretizing space, time, matter and forces. Integer operations are used exclusively throughout the computation. The physical space is a two dimensional hexagonal lattice, where the molecular objects occupy the sites of the lattice. The time is defined as synchronically performed update steps and is driven by an external clock.

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The Lattice Molecular Automata is designed in the spirit of the Lattice Gas Automata [11] and is an extension of the Lattice Polymer Automata [12], which both proved to be capable of generating macroscopic effects only based on a discrete, microscopic system representation. The interaction rules in the LMA emphasize especially a correct physical representation of molecular dynamics. They consider a variety of different molecular type specific interactions, as they are also implemented in classical force field models (and which in some ways are analogous to interaction site models [13]).

## 1.2 Discrete Representation of Molecular Systems

The Lattice Molecular Automata, introduced in this paper, is a novel simulation environment suited to handle large scale molecular self-assembly problems.

by extended, continuous force fields at the level of each atom. However, these methods are not capable to simulate large scale molecular systems over a long enough time scale, which is necessary for the treatment of molecular self-assembly systems. This failure is on the one hand based on insufficient computational power given the (atomic) level of description and on the other hand on the closed form (differential equation) description[10].