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Abstract	Lattice-gas cellular automata (LGCA)

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Lattice-Gas Cellular Automaton Models for Biology

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Synonyms

Lattice-gas cellular automata (LGCA)

Definition

A lattice-gas cellular automaton (LGCA) is a spatial modeling framework to analyze collective spatiotemporal behavior emerging in interacting and migrating cell populations, i.e., ▶ spatiotemporal pattern formation. LGCA represents a class of ▶ cellular automata whose structure facilitates mathematical analysis. Implementing movement of individuals in synchronous-update cellular automaton models is not straightforward, as one site in a lattice can typically only contain one individual, and consequently movement of individuals can cause collisions when two individuals want to move to the same empty site. In a lattice-gas cellular automaton model, this problem is avoided by having separate channels for each direction of movement and imposing an exclusion principle (Fig. 1). The movement steps are alternated with interaction steps, in which processes affecting cell number, e.g., birth and death can be implemented by specifying appropriate transition probabilities. The lattice-gas method allows for a clear separation of movement and interaction effects. The lattice-gas idea originates from physics, where it has been used for describing macroscopic gas and fluid dynamics, through implementing simple local interactions. Notwithstanding the abstract nature of the local rules, often the overall macroscopic behavior of the system can be approximated very well if averages over larger spatial scales are considered (Wolf-Gladrow 2000).

For a number of LGCA models, a corresponding lattice-Boltzmann approximation has been derived to analyze the emergence of spatiotemporal patterns (Deutsch and Dormann 2005). The idea behind the lattice-Boltzmann (mean-field) approximation is the reduction of the description of a system with many interacting individuals (many degrees of freedom), such as the LGCA, to the level of an effective, average description for the behavior of a single individual (few degrees of freedom). Assuming finite diffusion strength and based on the spatiotemporal mean-field description of the interaction process, one can often calculate the corresponding macroscopic partial differential equation by means of a Chapman-Enskog expansion technique (Wolf-Gladrow 2000). For example, from the mean-field partial differential equation for a migration and proliferation process, one can derive important macroscopic observables of biological growth, such as the total number of particles, the per capita growth rate, and the invasion speed, and reveal their dependence on the microscopic growth and transport parameters (Hatzikirou et al. 2010a).

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Characteristics

Biological organisms are complex systems characterized by ▶ collective behavior emerging out of the interaction of a large number of components (molecules and cells). In complex systems, even if the basic and local interactions are perfectly known, it is possible that the global (collective) behavior obeys new laws that are not obviously deduced from the individual properties. Only an understanding of the dynamics of collective effects at the molecular and cellular scale allows answers to biological key questions such as: What enables ensembles of molecules to organize themselves into cells? How do ensembles of cells create tissues and whole organisms? Key to solving these problems is the design and analysis of appropriate mathematical models of spatiotemporal pattern formation. More and more evidence has been provided of how populations of interacting and migrating cells can contribute in a self-organized manner to the formation of order in a developing organism. It has been realized that particular type of both the cell interaction and the migration are crucial, and that various combinations allow for a wide range of patterns. Lattice-gas cellular automata (LGCA) can model the interplay of cells with each other and their heterogeneous environment (Deutsch and Dormann 2005). These models describe interaction at a cell-based (microscopic) scale. Cell-based models (see also "▶ Cellular Potts Models," de Back et al., and "▶ Interacting Cell Systems," Voss-Böhme and Deutsch, this encyclopedia) are required to extract the organization principles of interacting cell systems down to length scales of the order of a cell diameter in order to link the individual (microscopic) cell dynamics with a particular collective (macroscopic) phenomenon.

Model Structure

Formally, a *lattice-gas cellular automaton* is defined as a tuple $(\mathcal{L}, \mathcal{E}, \mathcal{N}^I, \mathcal{R})$ with:

- *Velocity channels* $c_i \in \mathbb{R}^d$, $i = 0,\ldots, b-1$, where $b \in \mathbb{N}$ is fixed
- *Rest channels* $c_i \in \{0\}^d \subset \mathbb{R}^d$, $i = b,\ldots,\tilde{b}-1$ with a fixed $\tilde{b} \in \mathbb{N}$, $\tilde{b} \geq b$
- A set $\mathcal{L} = \left\{ r | r = \sum_{i=0}^{b-1} a_i c_i \text{ with } a_i \in X \right\} \subset \mathbb{R}^d$ called a *regular lattice* of dimension $d \in \mathbb{N}$, with $X = \mathbb{Z}$ or $X = [0, a] \subset \mathbb{Z}$ (with boundary conditions)
- A finite set of *states* $\mathcal{E} \in \{0,1\}^{\tilde{b}}$
- A *neighborhood of interaction* $\mathcal{N}^I = \left\{ e | e = \sum_{i=0}^{b-1} a_i c_i \text{ with } a_i \in Y_i \right\} \subset \mathbb{R}^d$ with $Y_i \subset X$ and $|Y_i| < \infty$, $i = 0,\ldots, b-1$
- A *local transition rule* $\mathcal{R}$

While the lattice $\mathcal{L}$ can be infinite, the neighborhood of interaction $\mathcal{N}^I$ has to be finite. For example, an infinite rectangular lattice in two dimensions with the Moore neighborhood as the neighborhood of interaction can be obtained by setting $X = \mathbb{Z}$, $b = 4$, $c_0 = (1,0)^T$, $c_1 = (-1,0)^T$, $c_2 = (0,1)^T$, $c_3 = (0,-1)^T$ for the velocity channels and $Y_0 = Y_1 = Y_2 = Y_3 = \{1\}$. The transition rule $\mathcal{R}$ is stochastic and specifies the transition probability between states. Each channel is either occupied or empty. The configuration at a node $r \in \mathcal{L}$ is given by:

$$\eta(r) := (\eta_0(r), \ldots, \eta_{\tilde{b}-1}(r)) \in \mathcal{E} = \{0,1\}^{\tilde{b}}, \eta_i(r) \in \{0,1\}, i = 0,\ldots,\tilde{b}-1$$

$\eta_i(r) = 1$ indicates that channel i at node r is occupied, while $\eta_i(r) = 0$ indicates an empty channel (Fig. 2). Au1

Dynamics

The time evolution of a lattice-gas cellular automaton is given by repeated application of the local transition rule $\mathcal{R}$, which is divided into two subsequently executed steps: an *interaction* step and a *migration* step. During both steps the whole lattice is updated synchronously. The *interaction* step assigns a new configuration $\eta_i^I(r) \in \mathcal{E}$ to node $r \in \mathcal{L}$ with probability $P\left(\eta_{\mathcal{N}_r} \to \eta^I(r)\right)$ depending on the previous configurations at r and the previous configurations $\eta_{\mathcal{N}_r}\left\{\eta(r') | r' \in \mathcal{N}_r^I\right\}$ in the neighborhood of interaction $\mathcal{N}_r^I = \{r + e | e \in \mathcal{N}^I\}$ of r. During the migration step all cells move to the corresponding velocity channels in the respective neighboring nodes, i.e., the new configuration $\eta^M \in \mathcal{E}$ is obtained by $\eta_i^M(r + c_i) = \eta_i(r)$, $i = 0,\ldots,\tilde{b}-1$.

Applications

LGCA models have been developed to analyze spatiotemporal pattern formation in microorganisms, cell cultures, and populations of cells in developing organisms (Deutsch and Dormann 2005; Börner et al. 2006; Moreira and Deutsch 2004). In particular, LGCA model modules (a simulation platform containing various LGCA "model modules" with biological motivations can be found at www.biomodeling.info) have been designed for random walk, differential adhesion, contact guidance, hapto- and chemotaxis, as well as for various growth and death processes (Deutsch and Dormann 2005).

Deciphering the principles of collective cell behavior is especially important for a better understanding of tumor growth and invasion and might allow to develop new therapy concepts. Besides more and more molecular investigations, mathematical modeling of selected aspects of tumor growth has become attractive within the last years (e.g., Anderson and Quaranta 2008). Cellular automaton models have been suggested for various aspects of tumor growth (Dormann and Deutsch 2002; Moreira and Deutsch 2002). In particular, simulations and analysis of appropriate LGCA models permit to characterize different growth and invasion scenarios (Hatzikirou et al. 2010b). A further important motivation for a discrete cell-oriented approach is that in cancerous systems, behavior often depends on fluctuations at the individual cell level, for example, at the front of invading tumors and during metastases formation. Obviously, corresponding mathematical cancer models have to be of a discrete nature and LGCA models are promising candidates.

Cross-References

- ▶ Cellular Automata
- ▶ Cellular Potts Model
- ▶ Collective Behavior
- ▶ Interacting Cell Systems
- ▶ Spatiotemporal Pattern Formation

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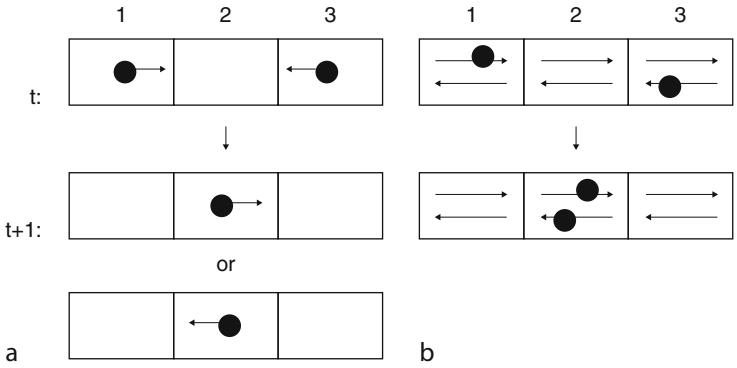
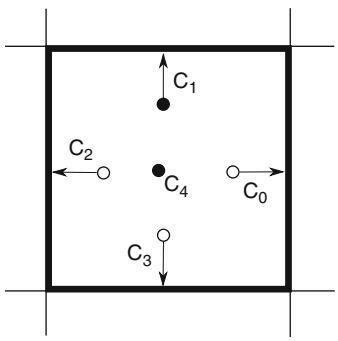
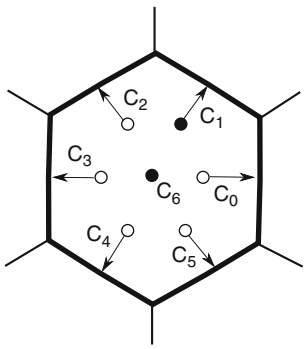


Lattice-Gas Cellular Automaton Models for Biology, Fig. 1 Movement in (**a**) a simple one-dimensional cellular automaton model (with just two states "empty" and "occupied"), and (**b**) in a corresponding lattice-gas cellular automaton model. *Filled circles* indicate occupied sites and channels, respectively. In the cellular automaton two individuals, from position 1 and 3, intend to move to position 2, causing a "collision", as a single site can only contain one individual. As a result, an additional rule has to be implemented that governs which of the two possible configurations arises. In contrast, in the lattice-gas simulation, each movement direction refers to a separate channel, and thus collisions are impossible. The result of the movement step ($t + 1$) will be that both channels in position 2 will be occupied





Lattice-Gas Cellular Automaton Models for Biology, Fig. 2 *Nodes of a rectangular and a hexagonal two-dimensional lattice*. There are four velocity channels c_0, c_1, c_2, c_3, and one rest channel c_4, and six velocity channels c_0, c_1, c_2, c_3, c_4, c_5, and one rest channel c_6, respectively. *Filled circles* denote occupied channels

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