Cellular Automata for Reaction-Diffusion Systems

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Abstract

Two classes of cellular automata for reaction-diffusion systems are presented. The first type, reactive lattice gas automata, realize diffusion through a random walk of particles on a lattice, while the second class is based on a local average, and closely related to finite difference schemes. The details of the reactive dynamics can either be derived from microscopic considerations (collision and reaction probabilities), or systematically constructed from the desired macroscopic reaction rate laws without regard to an underlying microscopic mechanism. For quantitatively correct modelling, the CA usually needs to be probabilistic, but in some cases a deterministic version proves sufficient.

Reactive Lattice Gas Automata

Reaction-diffusion systems are described by a set of partial differential equations of the form

$$\frac{\partial x_i(\mathbf{r},t)}{\partial t} = D_i \nabla^2 x_i(\mathbf{r},t) + f_i\Big(\{x_j(\mathbf{r},t)\}\Big) \tag{1}$$

where ∇^2 is the spatial Laplacian, and the functions f_i are the (usually nonlinear) reactive terms that depend on several different reactive species x_i.

In real systems, diffusion comes from the overall effect of many molecules executing independent random movements. The first CA method is closely related to the mechanism by which diffusion appears in real systems. We replace molecules by idealized particles and let these particles execute independent random walks on a regular lattice. These automata are usually called reactive lattice gas automata [1, 2, 5, 3].

The cellular automaton evolves on a square lattice on which particles propagate in two dimensions, with nearest neighbor interactions only.

Each particle has associated a velocity, which indicates the direction and distance the particle will move in one time step. In each cell, we allow at most one particle with each of five velocities, so that the state of a cell can be encoded with five bits, each of them indicating the presence of a particle with a particular velocity.

The transition rule is divided into two (later three) parts: Each time step consists of a propagation step (P) followed by a redistribution step (R).

Later we insert a "chemical" reactive step (C) after the propagation step. During the propagation step, the particles (bits representing the state) are copied from the respective neighbors so that each particle is displaced according to its velocity. In the second part, the redistribution step, the elastic collisions in real system are simulated, which lead to a randomization of the particle velocities. In the CA, we simply assign a new random velocity to each particle, taking into account the exclusion principle. This means that on a node with k particles, we have to choose one out of the $\binom{5}{k}$ possible configurations with the same number of particles. There is no interaction with the neighbors at this step, since all interaction takes place through the propagation step. The repeated application of the propagation and the redistribution steps leads to a random walk for each particle, since each particle makes a step of distance one (or zero) in a random direction at each time step.

The reactive part of the cellular automaton with diffusing particles couples the lattices for different species. This step usually needs to be probabilistic. Like the redistribution step, this step is also local to each node. Given that on one node there are α_i particles of species i, we replace these by β_i particles with probability $A(\{\alpha\},\{\beta\})$ (with $\{\alpha\}$ we denote the vector of values α_i for all i). All the details of the reactive dynamics lie in the construction of these probabilities.

One possibility for the construction of the probabilities is to start from a microscopic view: We describe the reactions we want to model as a list of reactive steps

$$\sum_i n_{u,i} X_i \xrightarrow{k_u} \sum_i m_{u,i} X_i. \tag{2}$$

The probability of changing a node with configuration $\{\alpha\}$ to configuration $\{\beta\}$ is set to

$$A(\{\alpha\},\{\beta\}) = V\Delta t \sum_u k_u \prod_i \frac{\alpha_i\,!}{(\alpha_i - n_{u,i})\,!}\,\frac{(V-n_{u,i})!}{V!}, \tag{3}$$

where $V = 5$ in our case.

Moving Average Cellular Automata

We now present a second class of cellular automata [4, 5] which models diffusion and reaction from a purely macroscopic point of view. For the diffusive part, we use a modified finite difference scheme, while for the reactive part we use probabilistic rules.

The operation

$$x(r, t+\Delta t) = \frac{1}{2R+1} \sum_{i=-R}^{R} x(r + i\,\Delta r, t) \tag{4}$$

leads to diffusive behavior with $D = \frac{R(R+1)}{6}\frac{\Delta r^2}{\Delta t}$. This local sum operation can be efficiently performed using a moving average technique. The result of this convolution operation applied to $x(\mathbf{r},t)$ is approximately

$$\Phi_D(x(\mathbf{r},t)) = x(\mathbf{r},t) + \tilde{D}\nabla^2 x(\mathbf{r},t). \tag{5}$$

We define the operator for the reactive part as

$$\Phi_R(c_0 x) = x(\mathbf{r},t) + \Delta t f(x(\mathbf{r},t)). \tag{6}$$

As defined, the output of operator Φ_R is not an integer number. We introduce another operator Φ_T for truncation, which takes the real numbers which result from operator Φ_R and produces an integer. The complete dynamics of the CA is given by $\Phi_T \circ \Phi_R \circ \Phi_D$.

For the truncation operator we have many choices, the most useful being

$$\Phi_T(x) = \begin{cases} \lfloor x \rfloor & \text{with probability} \quad 1-p \\ \lfloor x \rfloor + 1 & \text{with probability} \quad p = x - \lfloor x \rfloor. \end{cases} \tag{7}$$

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