A New Class of Cellular Automata for Reaction-Diffusion Systems

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We introduce a new class of cellular automata to model reaction-diffusion systems in a quantitatively correct way. The construction of the CA from the reaction-diffusion equation relies on a moving average procedure to implement diffusion, and a probabilistic table-lookup for the reactive part. The applicability of the new CA is demonstrated using the Ginzburg-Landau equation.

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Cellular automata models have been used in many applications to model reactive and diffusive systems [1,2]. Most uses of cellular automata (CAs) can be classified into one of four approaches: (i) Ising-type models of phase transitions; (ii) lattice gas models (the lattice gas method was initially developed to model hydrodynamic flows and has been extended in many directions [3,4]); (iii) systematic investigation of the behavior of CAs by investigating *all* rules of a certain class (e.g., all possible rules for one-dimensional automata with two states and nearest neighbor interaction) [1]; and (iv) qualitative discrete modelling (including operational use of CAs as an alternative to partial differential equations (PDEs) [5]). These models are generally based on qualitative rather than quantitative information about the system to be modelled. A CA is constructed which preserves the qualitative features deemed most relevant and it is then investigated (The lattice gas methods were also developed along these lines [6]). Existing CA models for reaction-diffusion systems [7–11] fall into the category (iv), i.e., they show qualitatively "correct" behavior and are restricted to certain reaction-diffusion (R-D) models and certain types of phenomena. This is the main criticism of experimentalists and researchers working with partial differential equation models, who search for quantitative predictions. In this letter we describe a class of CAs which is suitable for modelling many reaction-diffusion systems in a quantitatively correct way. The new CAs are operationally more efficient than the reactive lattice gas methods, which also achieve quantitative correctness. We first describe the construction of the new class of CAs; then we present the automaton using the Ginzburg-Landau equation as an example.

The main idea behind this class of CAs is careful discretization. Space and time are discretized as in normal finite difference methods for solving the PDE's. Finite difference methods then proceed to solve the resulting coupled system of $N \times s$ ordinary differential equations (N points in space, s equations in the PDE system) by any of a number of numerical methods, operating on floating point numbers. The use of floating point numbers on computers implies a discretization of the continuous variables. The errors introduced by this discretization and the ensuing roundoff errors are often not considered explicitly, but assumed to be small because the precision is rather high (8 decimal digits for usual floating point numbers). In contrast, in the CA approach, all variables are explicitly discretized into relatively small integers. This discretization allows the use of lookup tables to replace the evaluation of the nonlinear rate functions. It is this table lookup, combined with the fact that all calculations are performed using integers instead of floating point variables, that accounts for an improvement in speed of orders of magnitude on a conventional multi-purpose computer. The undesirable effects of discretization are overcome by using probabilistic rules for the updating of the CA.

The state of the CA is given by a regular array of concentration vectors $\mathbf{y}$ residing on a d-dimensional lattice. Each $\mathbf{y}(\mathbf{r})$ is a s-vector of integers (s is the number of reactive species). For reasons of efficiency, and to fulfill the finiteness condition of the definition of cellular automata, each component $\mathbf{y}_i(\mathbf{r})$ can only take integer values between 0 and $\mathbf{b}_i$, where the $\mathbf{b}_i$'s can be different for each species i. The position index $\mathbf{r}$ is a d-dimensional vector in the CA lattice. For cubic lattices, $\mathbf{r}$ is a d-vector of integers.

The central operation of the automaton consists of calculating the sum

$$\tilde{\mathbf{y}}_i(\mathbf{r}) = \sum_{\mathbf{r}' \in N_i} \mathbf{y}_i(\mathbf{r} + \mathbf{r}') \tag{1}$$

of the concentrations in some neighborhood N_i. The neighborhoods can be different for each species i. A neighborhood is specified as a set of displacement vectors, e.g. in two dimensions

$$N_{5-\text{star}} = \left\{ \binom{0}{0}, \binom{1}{0}, \binom{0}{1}, \binom{-1}{0}, \binom{0}{-1} \right\} \tag{2}$$

or

$$N_{1-\text{square}} =$$