Physica D 311–312 (2015) 1–16

Contents lists available at ScienceDirect

Physica D

journal homepage: www.elsevier.com/locate/physd

Cellular non-deterministic automata and partial differential equations

D. Kohler [a,b,*], J. Müller [a,c], U. Wever [b]

[a] Technische Universität München, Center for Mathematics, Boltzmannstr. 3, 85748 Garching/Munich, Germany

[b] Siemens AG, Corporate Technology, Otto-Hahn-Ring 6, 81730 Munich, Germany

[c] Helmholtz Zentrum München, Institute of Computational Biology, Ingolstädter Landstr. 1, 85764 Neuherberg, Germany

HIGHLIGHTS

- Cellular non-deterministic automata (CNDA) extend the concept of cellular automata.
- CNDA are defined in the spirit of non-deterministic automata theory.
- The dynamical behavior of a CNDA can be analyzed with deterministic superautomata.
- A CNDA can be embedded in a deterministic cellular automaton.
- CNDA can be used to approximate dynamics of certain partial differential equations.

ARTICLE INFO

Article history:
Received 21 January 2014
Received in revised form
31 July 2015
Accepted 3 August 2015
Available online 11 August 2015
Communicated by T. Sauer

Keywords:
Cellular automata
Partial differential equations
Asymptotic dynamics
de Bruijn states
Fisher–KPP equation

ABSTRACT

We define cellular non-deterministic automata (CNDA) in the spirit of non-deterministic automata theory. They are different from the well-known stochastic automata. We propose the concept of deterministic superautomata to analyze the dynamical behavior of a CNDA and show especially that a CNDA can be embedded in a deterministic cellular automaton. As an application we discuss a connection between certain partial differential equations and CNDA.

1. Introduction

On the one hand, spatial dynamical processes are mostly formulated as partial differential equations (PDE). As it is often difficult to obtain satisfactory analytical insight in practice, numerical schemes are applied. But despite the power of and recent progress in numerics, its practical use often encounters efficiency problems.

On the other hand, the theory of deterministic cellular automata (CA) evolved as an efficiently implementable description of spatial dynamical processes [1–3]. They are discrete in time, space and state space, and consist of spatially shift-invariant and local evolution rules [4,5]. Stochastic versions have also been introduced [6,7], which are similar to particle systems [8,9]. Well-known applications range from Conway's Game of Life [10] over excitable media [11] or biological pattern formation [6] to fluid dynamics through lattice–gas cellular automata and lattice Boltzmann methods [12]. Moreover, agent models on the basis of CA are very popular with applications in city [13] or society [14] modeling and crowd control [15].

Although also CA models carry certain drawback, it thus seems promising to develop a simplified description of a PDE in the discrete setup of CA. The goal is to derive an easy system that can be handled, simulated and – up to a certain degree – analyzed in a simpler way than the original PDE. Some approaches have been developed for the transition from state-continuous to state-discrete systems recently. Time-continuous dynamical systems on continuous state space can be studied by symbolic dynamics [16] or approximated by time-discrete Markov chains on finite state space [17]. This technique has led to the powerful tools of set oriented numerics [18,19], which is especially useful to study ergodic

* Corresponding author at: Technische Universität München, Center for Mathematics, Boltzmannstr. 3, 85748 Garching/Munich, Germany.
E-mail addresses: dominic.kohler@mytum.de (D. Kohler), johannes.mueller@mytum.de (J. Müller), utz.wever@siemens.com (U. Wever).

http://dx.doi.org/10.1016/j.physd.2015.08.001
0167-2789/

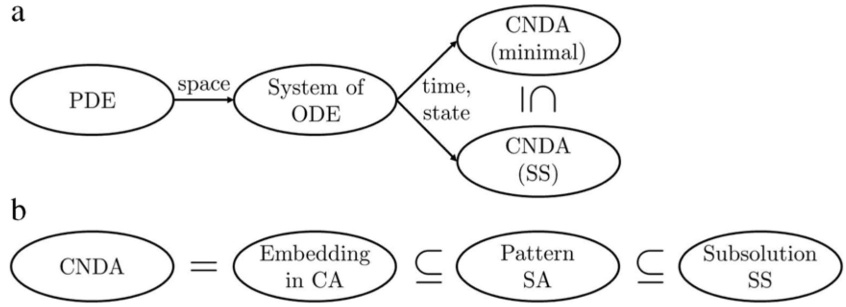

Fig. 1. (a) Space, time and state are discretized to describe the dynamics of a PDE by the dynamics of a CNDA. In many cases it is hard to determine the smallest possible CNDA and one ends up with a bigger CNDA which already carries less information. (b) A CNDA is covered by its SS of decreasing precision, see Section 4 for details.

theory, asymptotic dynamics and optimal control [20,21]. Alternative discretizations use information about special behavior of the continuous-state system [22] or have been discussed in the context of interval arithmetic [23] and for probabilistic graphical models with continuous states [24]. People have even argued in favor of a reformulation of physical laws in a discrete language [25,26]. Approaches for the specific transition from PDE to CA include ultradiscretization [27,28] and a probabilistic method [29]. We aim to contribute to this topic from another angle.

The idea is to dismiss information stepwise, see Fig. 1(a): first we use a method of line [30] to go from a PDE on $\mathbb{R}$ to a countable system of ordinary differential equations (ODEs); we replace $\mathbb{R}$ by $\mathbb{Z}$ by space discretization. Next we discretize the coupled ODEs in time and state by a variant of the set oriented methods for dynamical systems. The outcome is interpreted as a cellular non-deterministic automaton (CNDA) in the spirit of non-deterministic automata theory [31]: the transition of a state in one site is not deterministically determined by a configuration in the neighborhood, we only know a set of possible next states. This is a consequence of the second step of simplification and information reduction. In [32] we add transition probabilities to the possible image states and thus develop a method for uncertainty propagation. In contrast, the focus of this work is on the basic non-deterministic aspect in the context of CA theory.

We suggest to analyze such CNDA with supersystems (SS), especially by embedding them in or covering them with deterministic cellular superautomata (SA), see Fig. 1(b). This allows to approximate their dynamical behavior with the standard theory of CA at the cost of losing – in a controlled way – further information. One of these SS, the pattern SA, can be extended to the probabilistic setup in [32]. However, the work at hand is more general and also introduces and categorizes other approximation ideas. It depends very much on the system and the details of the whole procedure whether the SS reveals the essential features of the initial PDE. The method is chosen in such a way that it is always possible to construct a region covering the solution of the ODE. However, if the information loss is too high, the outcome may be trivial in the sense that it does not rule out most dynamical patterns but accept almost all patterns as possible structures.

The paper is structured as follows. In Section 2 we review some basic concepts of the theory of CA and dynamical systems to settle a notation, before we abstractly introduce and discuss CNDA in Section 3. Section 4 is concerned with the general analysis of CNDA with SS and SA. Then we show in detail in Section 5 how a CNDA may be constructed from a PDE as sketched above. We use the Fisher–KPP equation [33], which is central in the theory of reaction–diffusion processes [34], as a prototypical example in order to obtain some practical insight into the developed theory. Finally we conclude our results in Section 6.

2. Notation: Cellular automata and dynamical systems

In this section we review some basic concepts from cellular automata (CA) and dynamical systems theory to settle a notation.

2.1. Cellular automata

Let $(G, \cdot)$ be a finitely generated group with generators $\{\tau_1, \dots, \tau_n\}$, and E a finite set. G can be interpreted as the set of vertices of an associated graph, the Cayley graph, and is therefore in our context called a *grid* with *grid sites* $g \in G$. We write E^H for the set of all functions from $H \subseteq G$ to E and $\bar{e}_H$ for the function which is constantly $e \in E$ on H. When defining a $\varphi \in E^{\mathbb{Z}}$ explicitly we use the notational convention that the first written element of E after the dots always is the one at site $j = 0$. A *shift operator* is a mapping $\sigma_g : E^G \to E^G$, $\sigma_g(\varphi)(h) = \varphi(g \cdot h)$ for $g, h \in G$.

Definition 2.1. (i) A *(deterministic) cellular automaton (CA)* is a tuple (G, U, E, f_0) with G and E as above and $U = \{0, \tau_i^{\pm 1} \mid i = 1, \dots, n\}$ the *neighborhood* of the unit element $0 \in G$. $f_0 : E^U \to E$ is a *local function* that induces the *global function* $f : E^G \to E^G$, $\varphi \mapsto f(\varphi)$ with

$$f(\varphi)(g) = f_0(\sigma_g(\varphi)|_U)$$

for $g \in G$. The *(deterministic) trajectory starting with* $\varphi_0 \in E^G$ is given by the sequence $(\varphi_n)_{n\in\mathbb{N}}$, where $\varphi_n = f(\varphi_{n-1})$ for $n \in \mathbb{N}^+$.

(ii) If there is exactly one marked element $0 \in E$ with $f_0(\bar{0}_U) = 0$, the CA is said to have a *resting state*.

(iii) For finite $H \subset G$, $h \in E^H$ is said to be a *Garden of Eden pattern*, if there are no states $\varphi, \psi \in E^G$ with $\varphi|_H = h$ and $\varphi = f(\psi)$ [35].

Understanding the restriction $\varphi|_{g\cdot U}$ as a function with domain U, it holds that $\sigma_g(\varphi)|_U = \varphi(g \cdot U) = \varphi|_{g\cdot U}$ and therefore $f_0(\sigma_g(\varphi)|_U) = f_0(\varphi|_{g\cdot U})$.

Although many definitions and results may be extended to more general groups, we restrict ourselves mostly to the group $(\mathbb{Z}, +)$ in the following. It will turn out that this is sufficient to apply our ideas to the simulation of partial differential equations in one spatial dimension. We call $|U| = m + n + 1$ the *length* of a set $U = \{-m, \dots, n\}$ such as the neighborhood, where $m, n \in \mathbb{N}$. In case of E carrying an order $\leq$, $\varphi \in E^{\mathbb{Z}}$ is called *monotonic* if $\varphi(i) \leq \varphi(j)$ for all $i \leq j$ or if $\varphi(i) \geq \varphi(j)$ for all $i \leq j$, where $i, j \in \mathbb{Z}$.

Definition 2.2. Let $\varphi, \psi \in E^{\mathbb{Z}}$. The *Cantor metric* d_C is given by $d_C(\varphi, \psi) = 0$ if $\varphi = \psi$ and $d_C(\varphi, \psi) = \frac{1}{1+i}$ otherwise, where i is the least non-negative integer such that either $\varphi(i) \neq \psi(i)$ or $\varphi(-i) \neq \psi(-i)$. The induced topology is called the *Cantor topology*.