

# Qualitative and Quantitative Cellular Automata from Differential Equations

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**Abstract.** We give a synthetic and formalized account of relationships between cellular automata (CA) and differential equations (DE): Numerical schemes and phase portraits analysis (via cell-to-cell mappings) can be translated into CA, and compositions of differential operators and phase portraits induce CA compositions. Based on DE, CA can be tuned according to discretization parameters so that faithful CA sequences can be built describing qualitative as well as quantitative solutions.

## 1 Introduction

Cellular automata (CA) are parallel context-sensitive rewriting processes which are used as computation models and as effective ways of simulating physical, chemical or biological phenomena [20, 3, 5, 26]. With this respect, CA have been mostly considered as tools giving qualitative information, but quantitative information has also been shown reachable [7, 6, 2, 24, 23]. This paper generalizes this fact by setting up in a precise way relationships that exist between CA and (systems of) ordinary and partial differential equations (DE). These relationships show how the CA-DE pair can be seen as a generic model to gradually go from qualitative information to quantitative information and vice versa.

We first recall how CA are related to *explicit numerical schemes* to solve DE. Next, we show how *integrated phase portraits of autonomous DE* are transformed into CA (making the link with *cell-to-cell mapping theory* [9]). Compositions of CA can also be based on their relationships with DE : CA are coupled as are differential operators in *splitting techniques* classically used to solve DE [27]; CA can also be coupled as are *invariant regions* of DE phase portraits. The finer (resp. coarser) the involved discretizations in a resolution of a DE, the more quantitative (resp. qualitative) the computations of the induced CA. By tuning discretization levels, qualitative descriptions can be related in a controlled way to quantitative descriptions, yielding what we call here *faithful CA sequences*. Looking for the first terms of these sequences, that is, looking for the simplest meaningful CA, becomes a way of minimizing time and space complexity, but also a way of understanding the model from a “*Kolmogorov complexity point-of-view*”. Based on DE, this search for minimal CA can be driven by studying how and which features are preserved, deformed, smoothed or swept out. In particular, we discuss the existence of *spurious* and *eluded fixed points*, one of the main features indicating that maximum coarseness has been reached.

## 2 Basics

A *cellular automaton* (CA) is a simple context-sensitive rewriting mechanism for which the whole input is processed in parallel using a uniform rewriting rule. Here, we consider CA defined over *lattices* embedded in  $\mathbb{R}^n$ , i.e. additive subgroups of  $(\mathbb{R}^n, +)$  spanned by ordered sets of  $n$  independent vectors. A CA is a 4-tuple  $\mathcal{A} = (\mathcal{L}_n, \mathcal{Q}, N, \tau)$  where  $\mathcal{L}_n$  is a lattice in  $\mathbb{R}^n$  whose elements are the *cells*, and where  $n \geq 0$  is the CA *dimension*;  $\mathcal{Q}$  is a finite set of *states*;  $N : \mathcal{L}_n \rightarrow 2^{\mathcal{L}_n}$  is a *neighborhood* such that  $N(x) = \phi_x(N(x_0))$  where  $N(x_0)$  is a set of vectors in  $\mathcal{L}_n$  starting at  $x_0 \in \mathcal{L}_n$ , and  $\phi_x$  is a translation sending  $x_0$  to  $x$  ( $N$  is such that every  $x$  has the same form of neighborhood as  $x_0$ );  $\tau : \mathcal{Q}^{N(x_0)} \rightarrow \mathcal{Q}$  is a *local transition function*. A CA *configuration*  $f$  is a global state, that is, an element of  $\mathcal{Q}^{\mathcal{L}_n}$ . The transition function  $\tau$  is extended as a *global transition function*  $\tilde{\tau} : \mathcal{Q}^{\mathcal{L}_n} \rightarrow \mathcal{Q}^{\mathcal{L}_n}$  by applying  $\tau$  to each cell  $x$  as  $\tilde{\tau}(f)(x) = \tau(\phi_{-x} \circ f|_{N(x)})$ . Applying  $\tilde{\tau}$  once is called a *step*. A *run* of a CA is a sequence of consecutive steps starting at an *initial configuration*. Note that these definitions just differ from the classical ones by directly including an CA embedding into  $\mathbb{R}^n$ .

An *ordinary differential equation* (ODE) is  $F(t, u, \frac{du}{dt}, \frac{d^2u}{dt^2}, \dots, \frac{d^m u}{dt^m}) = 0$ , where the unknown function  $u$  is such that  $u(t) : \mathbb{R} \rightarrow Y$  where  $Y$  is a differentiable manifold called the *phase space* or the *state space*. A *partial differential equation* (PDE) is  $F(t, x_1, \dots, x_n, u, \frac{\partial u}{\partial t}, \frac{\partial u}{\partial x_1}, \dots, \frac{\partial^2 u}{\partial x_1 \partial x_2}, \dots) = 0$ , where the unknown function is such that  $u(t, x_1, \dots, x_n) : \mathbb{R} \times X \rightarrow Y$  where  $X$  is called the *domain*. Here,  $Y$  and  $X$  will be restricted to  $\mathbb{R}^n$ . We shall also only consider *initial-value problems* with exactly one solution, i.e. unique  $u(t, \cdot)$  with given prescribed values  $u(t_0, \cdot)$  at a given time  $t_0$ . When the phase space  $Y$  can be decomposed as a Cartesian product  $Y_1 \times \dots \times Y_p$ , one may consider *systems of DE* with an unknown function  $u = (u_1, \dots, u_p)$ .

A numerical method for solving a DE involves three discretization operations respectively applied to the source space of  $u$ , the phase space  $Y$ , and the differential equation itself: **(1)** Discretizations of the source space generally rely on embedded lattices. For example, regular discretizations of  $\mathbb{R}^2$  can be obtained from lattices  $\mathcal{L}_2 \subset \mathbb{R}^2$  spanned by two orthogonal vectors of norms  $\delta t$  and  $\delta x$  with an offset shift, i.e.  $\{(t, x) \in \mathbb{R}^2 | t = i\delta t + \sigma_t, x = j\delta x + \sigma_x, i, j \in \mathbb{Z}\}$ . **(2)** Discretizations of the phase space  $Y$  – henceforth denoted by  $Y_{disc}$  – are called *quantifications*. Regular discretizations can also be used here, but the most common ones are based on *floating-point numbers* which are non-regular finite quantifications. Sending  $Y$  to  $Y_{disc}$  is done by *quantification projection functions*. Quantifications and their projection functions lead to *round-off errors*. **(3)** Discretizations of the DE can be obtained by *finite difference schemes* where the differential operators are replaced by difference operators involving only points of the discretized source space (see e.g. [19]). For instance, consider  $\frac{du}{dt} = f(t, u)$  with  $u : \mathbb{R} \rightarrow \mathbb{R}$ . Let the source discretization be a lattice  $\mathcal{L}_1$  spanned by a  $\delta t$  vector. The so-called *Euler scheme* is based on the two first terms of the *Taylor sequence* of  $u$ , i.e.  $U(t_0 + \delta t) = U(t_0) + \delta t f(t_0, U(t_0))$ , where  $U$  is an approximation of  $u$ . Solving an initial value problem from  $u(t_0)$  for given  $\delta t$  and  $Y_{disc}$  is obtained by iterating this scheme: Denoting the  $i$ -th time point  $i\delta t$  by  $t_i$ , we

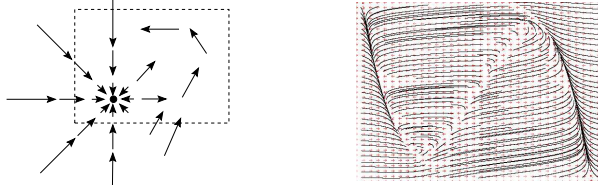
get  $U(t_{i+1}) = U(t_i) + \delta t f(t_i, U(t_i))$ ,  $i \geq 0$ . As another instance, consider the 2D heat PDE diffusion process  $\frac{\partial u}{\partial t} = K(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2})$  and a discretization of its source space spanned by vectors of respective norms  $\delta t, \delta, \delta$ . The *forward-time central-space* finite difference scheme is defined by  $U(t_{i+1}, x_j, y_k) = r(U(t_i, x_{j-1}, y_k) + U(t_i, x_{j+1}, y_k) + U(t_i, x_j, y_{k-1})) + (1-4r)U(t_i, x_j, y_k)$  where  $r = K\frac{\delta t}{\delta^2}$ . These two examples are *explicit numerical schemes*: approximations  $U$  of  $u$  are built after a map  $g$  such that:  $U(t_{i+1}) = g(U(t_i, \cdot), \dots, U(t_{i-m}, \cdot), t_i, \dots, t_{i-m})$ , with  $0 \leq m < \infty$ . In the case that a DE is *autonomous*, which means that the solutions do not depend on time, the scheme can be reduced to  $U(t_{i+1}) = g(U(t_i, \cdot), \dots, U(t_{i-m}, \cdot))$ . Note that a non-autonomous system can be made autonomous by adding the equation  $\frac{du_{p+1}}{dt} = 1$ . The following first relationship between CA and DE has been informally known for a long time (see e.g. [25]):

**Proposition 1.** (*Explicit methods and CA*). *Let  $F(u) = 0$  be a (system of) autonomous DE with  $u : \mathbb{R} \times \mathbb{R}^n \rightarrow Y$ ,  $n \geq 0$ . Let  $Y_{disc}$  be a finite quantification of  $Y$ , and let  $\mathcal{L}_1 \times \mathcal{L}_n$  be a discretization of  $\mathbb{R} \times \mathbb{R}^n$ . Then an explicit numerical scheme  $g$  for solving  $F$  according to these discretizations can be transformed in a CA  $(\mathcal{L}_n, Y_{disc}, N_g, g)$ , where  $N_g$  is defined by the points in  $\mathcal{L}_n$  used in  $g$ .*

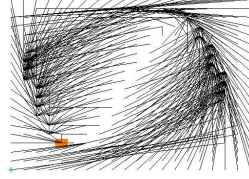
Euler schemes yield 0-dimensional CA (domain spaces are restricted to a single point)<sup>1</sup>. Heat diffusion processes in  $n$ -dimensions lead to  $n$ -dimensional CA.

There is another important way of relating DE to CA: When autonomous, a (system of) ODE has a solution space  $\mathbb{R} \times Y$  which can be projected without loss of information to the phase space  $Y$  as a vector field called *phase portrait*. This vector field can be integrated to obtain a *solution flow*. For a system of  $p$  autonomous ODE defined by  $\frac{du_i}{dt} = f_i(u_i)$  for which  $Y = \mathbb{R}^p$ , the phase portrait is  $\vec{v}(x_1, \dots, x_p) = (f_1(u_1(\cdot)), \dots, f_p(u_p(\cdot)))$ . For instance, *reaction phenomena* (see e.g. [14]) are captured by autonomous systems of ODE whose phase portraits involve swerving-like behavior around attractive singularities (see Fig. 1). One of these systems is the 2D *Fitzhugh-Nagumo equation* which describes spatial propagation of action potential impulses along the nerve axon by  $\frac{du_1}{dt} = (a - u_1)(u_1 - 1)u_1 - u_2$  and  $\frac{du_2}{dt} = \epsilon(u_1 - bu_2)$  with  $0 < a < 1$ ,  $b > 0$ ,  $\epsilon \in \mathbb{R}$ . One can discretize such DE by directly referring to their phase portraits: First, consider a regular discretization  $Y_{disc}$  of  $Y$ , and let  $\Phi$  be a numerical method to solve the DE with a fixed integration time  $\delta t > 0$ . From each point in  $Y_{disc}$ , we can integrate the equation by  $\Phi$  during  $\delta t$  and determine its ending point in  $Y_{disc}$ . The result is a relation in  $Y_{disc} \times Y_{disc}$ , generally studied under the name of *cell-to-cell mappings* [9]. Now, assume that  $Y$  includes *invariant bounded subdomains*, that is, regions  $\mathcal{R} \subset Y$  from which the solutions having initial points in  $\mathcal{R}$  are strictly contained in  $\mathcal{R}$  (a sufficient condition for invariance is that every vector of the vector field on the boundary  $\partial\mathcal{R}$  is tangent or entering  $\mathcal{R}$ ). Letting  $\mathcal{R}_{disc}$  be the discretization of  $\mathcal{R}$  rel. to  $Y_{disc}$ , the sub-relation  $\mathcal{R}_{disc} \times \mathcal{R}_{disc}$  is finite and defines a possible transition function  $\tau_\Phi$  of a 0D CA. For instance, in

<sup>1</sup> Such 0D CA  $(\{c\}, \mathcal{Q}, \{c\}, \tau)$  just define finite state paths over a single cell  $c$ . They mainly become of interest when composed with  $n$ D CA with  $n > 0$  (see p. 5).



**Fig. 1.** To the left, the general appearance of the phase portrait of a 2D reaction DE system. The framed region is more precisely represented to the right for a Fitzhugh-Nagumo equation with  $a = 0.1$ ,  $\epsilon = 0.005$ ,  $b = 4$ , together with some integral solutions.



**Fig. 2.** A CA of 400 states corresponding to the above invariant region (left of Fig. 1), i.e.  $[-0.39, 1.1] \times [-0.03, 0.16]$ , discretized by a  $20 \times 20$  grid and integrated by a 4th order Runge-Kutta method with time step  $\delta t = 20$  (200 steps of time length 0.1).

the case of the Fitzhugh-Nagumo equation, every bounded rectangular domain containing the parallelogram-like shape of the phase portrait (see Fig. 1) can be proved invariant [4, 16, 8].

**Proposition 2.** (*Phase portraits and CA*). Let  $F(u) = 0$  be a (system of) autonomous ODE. Let  $\mathcal{R} \subset Y$  be a bounded invariant region and let  $\mathcal{R}_{disc}$  be a regular discretization of  $\mathcal{R}$ . Let  $F(u) = 0$  be such that the solutions of the initial value problems starting from  $\mathcal{R}_{disc}$  exist and are unique, and let  $\Phi$  be a numerical scheme to approximate these solutions. Then there are zero-dimensional CA  $(\{c\}, \mathcal{R}_{disc}, \{c\}, \tau_\Phi)$  whose runs also approximate these solutions.

Note that unlike general *explicit schemes*,  $\Phi$  has no *a priori* limitations (e.g. *instability-prone* [19]) and can be chosen to be as precise as one wants. Prop. 2 has been already implicitly used to build ad-hoc CA for reaction-diffusion systems (see e.g. [7, 6, 2]), and also more explicitly [24].

### 3 DE Coupling and CA Compositions

An effective and direct way of coupling DE consists of adding differential operators. The simplest case is expressed as:  $\frac{\partial u}{\partial t} = F(u) = F_1(u) + \dots + F_m(u)$ . For instance, the full 2D Fitzhugh-Nagumo *reaction-diffusion* system includes a reaction part and a diffusion part:  $\frac{\partial u_1}{\partial t} = [(a - u_1)(u_1 - 1)u_1 - u_2] + K(\frac{\partial^2 u_1}{\partial x^2} + \frac{\partial^2 u_1}{\partial y^2})$

and  $\frac{\partial u_2}{\partial t} = \epsilon(u_1 - bu_2)$ . One can also add *drift components* [13], for instance wrt the  $x$  dimension:  $\frac{\partial u_1}{\partial t} = H(\frac{\partial u_1}{\partial x}) + [(a - u_1)(u_1 - 1)u_1 - u_2] + K(\frac{\partial^2 u_1}{\partial x^2} + \frac{\partial^2 u_1}{\partial y^2})$  and  $\frac{\partial u_2}{\partial t} = H(\frac{\partial u_2}{\partial x}) + [\epsilon(u_1 - bu_2)]$ . Many meaningful DE models can be designed following this composition technique (see e.g. [15]). Now, there exists a classical method to numerically solve such composed DE called *operator splitting* (or *fractional step method*) (see e.g. [27, 1]). This method relies on decomposing a DE into its pieces, where each piece is expected to be easier to solve. For instance, the simplest splitting for the above general equation  $F(u)$  is to solve the sub-equations  $\frac{\partial u}{\partial t} = F_j(u)$  for  $j = 1, \dots, m$  by distinct numerical schemes  $g_j$ , and to get solution approximations by their direct composition:  $U(t_{i+1}) = g_m(g_{m-1}(\dots(g_1(U(t_i), \dots))))$ . Composing such numerical operators in this way has a counterpart in the CA side:

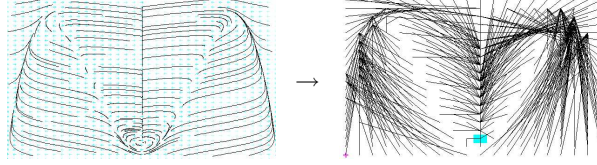
**Proposition 3.** (*Splittings and CA*). Let  $\frac{\partial u}{\partial t} = F(u) = F_1(u) + \dots + F_m(u)$  be a DE with  $u : \mathbb{R} \times \mathbb{R}^n \rightarrow Y$ . Let  $\mathcal{L}_1 \times \mathcal{L}_n$  be a discretization of  $\mathbb{R} \times \mathbb{R}^n$ , and let the DE be solvable by an operator splitting for which the sub-equations are  $\frac{\partial u}{\partial t} = F_j(u)$ ,  $j = 1, \dots, m$ . Assume the involved  $m$  numerical schemes can be transformed into  $m$  distinct CA over the same set of states, i.e.  $\mathcal{A}_j = (\mathcal{L}_{n_j}^{(j)}, \mathcal{Q}, N^{(j)}, \tau^{(j)})$  for  $j = 1, \dots, m$ , with  $n_j \leq n$ , and such that for each  $j$ , the lattice  $\mathcal{L}_n$  is partitioned into copies of  $\mathcal{L}_{n_j}^{(j)}$  according to the variable dimensions involved in the  $j$ -th equation. Then a corresponding CA  $(\mathcal{L}_n, \mathcal{Q}, N, \tau)$  is defined by sequentially applying the  $\mathcal{A}_j$ 's to  $\mathcal{L}_n$ , where  $\tau$  consists of applying  $\tau^{(j)}$  to each copy of  $\mathcal{L}_{n_j}^{(j)}$  in  $\mathcal{L}_n$ .

A special case occurs when some  $n_j = 0$  (i.e. the sub-equation is not a PDE): the corresponding CA is zero-dimensional and the partition of the global reference lattice  $\mathcal{L}_n$  consists of its single elements. Reaction-diffusion systems are classic instances taking advantage of the above composition process [7, 6, 24]: reaction terms are associated to 0D CA, and  $n$ D diffusion to  $n$ D CA.

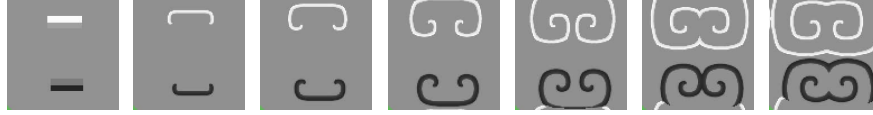
There is another way of coupling sets of (systems of) autonomous DE which relies on assembling invariant sub-regions of their phase portraits: Let  $\mathcal{R}$  be a region of  $\mathbb{R}^n$  (with non-empty interior), let  $\mathcal{R}_\epsilon = \{x \in \mathbb{R}^n \mid \exists y \in \mathcal{R}, d(x, y) < \epsilon\}$  where  $\epsilon > 0$  and  $d$  is the Euclidean metric, and let  $\mathcal{R}_{-\epsilon}$  be the region such that  $(\mathcal{R}_{-\epsilon})_\epsilon = \mathcal{R}$ . A *smooth characteristic function* wrt  $\mathcal{R}$  is a continuous monotonic function  $\psi$  such that  $\psi \equiv 1$  in  $\mathcal{R}_{-\epsilon}$ ,  $\psi \equiv 0$  in the complement of  $\mathcal{R}_\epsilon$  in  $\mathbb{R}^n$ , and  $\psi$  takes its values in  $[0, 1]$  for the other points. Consider  $M$  systems of autonomous DE  $\frac{du}{dt} = F_j(u)$  acting on the phase space  $Y$ , each of them associated to a function  $\psi_j$  whose regions  $\mathcal{R}_j$  have pairwise disjoint interiors. These systems can be composed by  $\frac{du}{dt} = F(u) = \psi_1 F_1(u) + \dots + \psi_M F_M(u)$ . This can also be reflected in the CA side:

**Proposition 4.** (*Phase portrait compositions and CA*). Consider a DE built according to the above composition technique. Assume there is a zero-dimensional CA  $(\{c\}, \mathcal{Q}^{(j)}, \{c\}, \tau^{(j)})$  corresponding to each region  $\mathcal{R}_j$ . Then the composed CA is defined by  $(\{c\}, \mathcal{Q}^{(1)} \cup \dots \cup \mathcal{Q}^{(M)}, \{c\}, \tau^{(1)} \circ \dots \circ \tau^{(M)})$ .

For instance, reaction equations one can be coupled by composing the invariant regions of their phase portraits. Indeed, let  $\phi_x$  denote a horizontal translation of



**Fig. 3.** To the left, the global invariant region of the phase portrait of a Fitzhugh-Nagumo “double reaction”. To the right, a corresponding CA with 400 states (a  $20 \times 20$  grid), built by the same integration method as in Fig. 2.



**Fig. 4.** A run of the CA obtained by composing the above CA (Fig. 3) and a diffusion CA. This run is sampled every 10 steps from 0 to 60 and only the values of  $u_1$  (horizontal dimension) are shown (the higher the value, the brighter the corresponding point of  $X$ ). As expected, the white waves have a higher frequency than the black waves.

along the  $x$ -axis, let  $\rho$  be the reflexion wrt the  $y$ -axis and let  $h_\alpha$  be a scaling with coefficient  $\alpha$ . Let us denote the Fitzhugh-Nagumo equation by  $Fitz$ . First, we translate it to the right:  $Fitz^{(1)} \equiv \phi_{x_1} \circ Fitz$  with  $x_1 \in \mathbb{R}^+$ . Second, the system  $Fitz^{(1)}$  can be reflected and scaled:  $Fitz^{(2)} \equiv h_{\alpha_1} \circ \rho \circ Fitz^{(1)}$  with  $\alpha_1 \in \mathbb{R}^+$ . If  $x_1 > 0$  is large enough, the invariant regions of  $Fitz^{(1)}$  and  $Fitz^{(2)}$  lie in each side of the  $y$ -axis, and they are disjoint except for their attractive fixed point (a case not impairing the composability). DE coupling is then applied by using characteristic functions  $\psi_1$  and  $\psi_2$  for their respective invariant regions:  $\frac{\partial u_i}{\partial t} = \psi_1(u_1, u_2) \cdot Fitz^{(1)}(u_1, u_2) + \psi_2(u_1, u_2) \cdot Fitz^{(2)}(u_1, u_2)$  (see Fig. 3). This “double reaction” can be transformed into a CA by composing the CA of each reaction. Note however that when used in a splitting, the invariant regions must be chosen so that all the involved CA are defined over the same set of states (cf. Prop 3). For instance, a double reaction CA composed with a diffusion CA needs a rectangular global invariant region containing a part of the  $y$ -axis. When this condition is satisfied, the resulting CA runs show two kinds of traveling waves living together, inducing spirals of two different sizes and frequencies (see Fig. 4).

## 4 CA Sequences and Tunability

The above constructions establish connections between DE and CA using specific numerical and composition schemes. However, not much has been said about their properties. One of the most important one is *convergence*: Let the source space be  $\mathbb{R}$ , and consider  $F(u) = 0$ . Let  $\{\mathcal{L}_1^k\}$  be a sequence of regular discretizations of  $\mathbb{R}$  spanned by  $\delta t_k$  with  $\delta t_k \rightarrow 0$  as  $k \rightarrow 0$ . A numerical scheme to solve

$F(u) = 0$  is *convergent* iff for every exact solution  $u$  wrt an initial condition and for every  $T > 0$ , the sequence of the computed solutions  $\{U_{\delta t_k}\}$  is such that:  $\max_{0 \leq i \leq T/\delta t_k} |U_{\delta t_k}(t_i) - u(t_i)| \rightarrow 0$ , as  $U_{\delta t_k}(t_0) \rightarrow u(t_0)$  and  $\delta t_k \rightarrow 0$ .

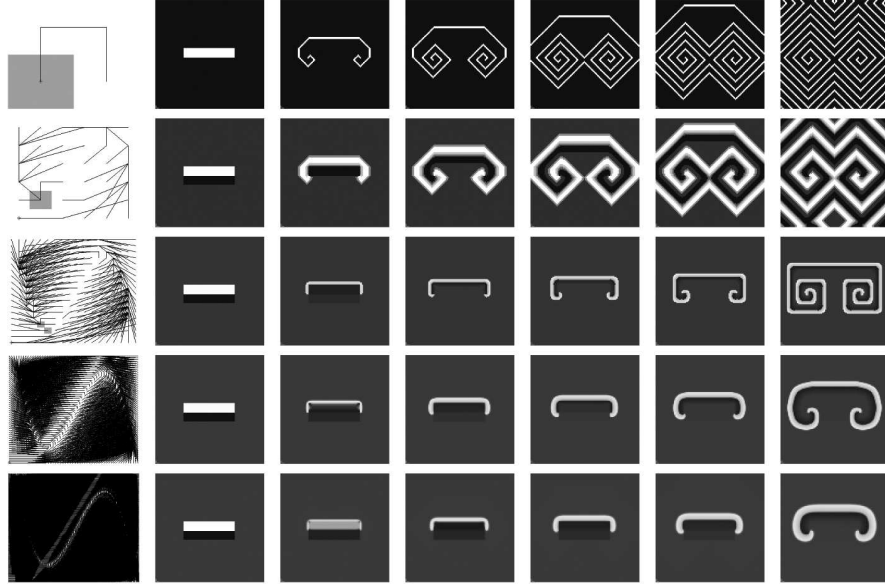
**Proposition 5.** (*Convergent numerical schemes and CA sequences*). Let  $F(u) = 0$  be a (system of) autonomous DE with  $u : \mathbb{R} \times \mathbb{R}^n \rightarrow Y$  and  $n \geq 0$ . Let  $g$  be any kind of convergent explicit numerical scheme to solve the DE. Then one can associate a CA sequence  $\{\mathcal{A}_i\}$  to  $g$  which is also convergent.

Let us discuss the case for which the source space is  $\mathbb{R}$ . According to their definition, CA need discretizations of the phase space  $Y$ , whereas usual convergence definitions – like the above one – do not include them. But clearly, if a discretization of  $Y$  does not evolve,  $|U_{\delta t_k}(t_i) - u(t_i)|$  could not in general go to zero as  $\delta t_k \rightarrow 0$ . Therefore, one must consider another sequence of finer and finer discretizations of  $Y$ . For the sake of simplicity, assume these discretizations are regular and spanned by  $\delta y_k$ . For each discretization of  $\mathbb{R}$  based on  $\delta t_k$ , there is a quantification projection function  $\rho_k$  sending  $U_{\delta t_k}$  to its quantified version  $U_{\delta t_k, \delta y_k}$  such that  $|\rho_k(U_{\delta t_k}) - U_{\delta t_k, \delta y_k}| < \delta y_k$ . Hence,  $\{U_{\delta t_k, \delta y_k}\}$  can be defined so as to converge to  $u$ . If the associated numerical scheme is explicit, one can translate this sequence into a convergent CA sequence  $\{\mathcal{A}_k\}$ , where the number of states of each  $\mathcal{A}_k$  is determined by  $\delta y_k$ .

Convergence gives a coherent way of tuning CA wrt the numerical discretization parameters. For example, Fig. 5 shows some terms of a CA sequence corresponding to a Fitzhugh-Nagumo reaction resolution. Accordingly, we use finer and finer discretizations of the invariant region of its phase portrait. The runs of the corresponding reaction-diffusion CA yield more and more quantitative features. Exact behaviors and shapes of the solutions are obtained, e.g. *curvatures of the isoclines* or *dispersion effects* [11, 6]. Note however that in the general case, convergence is not sufficient to ensure that a numerical scheme – and therefore a CA sequence – converges to the true DE solutions. Concepts as *consistency*, *well-posedness* and *stability* must also be considered (see e.g. [19]).

## 5 Faithfulness and Qualitativeness

The precedent section emphasizes a fundamental difference between CA and numerical methods: quantification of the phase space  $Y$  is an intrinsic part of a CA (a finite sets of states), whereas in numerical methods, quantification is either neglected or considered as a disturbing element. But coarse discretizations of  $Y$  may yield results still bearing the main features of the DE's solutions. Thus, we could not only find good solution approximations as discretizations become finer, we could also search for coarse discretizations of  $Y$  for which some qualitative aspects of the solutions are preserved. The first terms of a convergent CA sequence become important too. When all the terms of a convergent CA sequence generate some meaningful/qualitative features of the solutions of a DE, this sequence is said to be *faithful* to the DE. Faithfulness indicates how CA could enrich the concept of DE numerical computation by including the

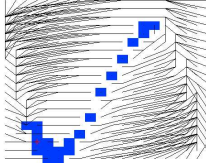


**Fig. 5.** In the left column, elements of a CA sequence for a Fitzhugh-Nagumo reaction (the representation is the same as in Fig. 2, and small gray rectangles indicate fixed points). From the top to the bottom, the region  $\mathcal{R}_{disc}$  has been discretized according to grids of resp. of  $2^2$ ,  $6^2$ ,  $18^2$ ,  $54^2$  and  $162^2$  points (multiplication by 3 preserves the offsets). To the right of each reaction CA is shown a run of the corresponding reaction-diffusion CA after 5, 10, 15, 20 and 40 steps. As the integration time  $\delta t$  of the reaction decreases (to be kept proportional to the cell size defined by the discretization and the quantification projection function, see Prop. 2), the wave frequency decreases too.

idea of reducing, minimizing, optimizing these computations, and not only by providing exact computations. The example given in Fig. 5 shows that faithful CA sequences exist, even for non-trivial cases like reaction-diffusion DE: traveling waves occur at very coarse discretization levels of the phase space. Spirals are just more square-like when the phase space is reduced to very few states.

Of course, the qualitative properties of a DE solution space are not easily described in a full general setting. Nevertheless, phase spaces contain some decisive features, like for instance in the autonomous case, *singularities* of their phase portraits – i.e. fixed and periodic points (see e.g. [10]). With this respect, when using coarse discretizations, two main problems may occur: *spurious fixed points* appear or real fixed points are *eluded*. To ensure faithfulness, a natural expected condition is to avoid these. In the case of ODE systems, determining the real fixed points requires to solve  $\frac{du_i}{dt}(x) = 0$ , for every  $i$ . In the Fitzhugh-Nagumo case, this amounts to solve  $(a - u_1)(u_1 - 1)u_1 = u_1/b$ . When the slope of the linear isocline is steep enough wrt the cubic isocline (e.g.  $a = 0.1$  and  $b = 4$ ), there is a unique fixed point at  $(0, 0)$ , and every solution finishes eventually at





**Fig. 6.** A CA for the same Fitzhugh-Nagumo reaction as in Fig. 2, but built with a too short integration time  $\delta t = 4$ : many spurious fixed points occur (gray rectangles).

$(0, 0)$  (no cycle exists). Associated CA can be built (cf. Prop. 2) so as to comply with these properties. When the integration time step  $\delta t$  is too short, spurious fixed points mainly occur on the cubic nullcline (see Fig. 6). Tuning  $\delta t$  wrt  $Y_{disc}$  has been important to obtain Fig. 5. Note that by continuity, some spurious fixed points may occur in a neighborhood of a real fixed point without much influence. One can also preserve fixed point types like being *attractive*, *repulsive*, *stable*, *unstable*, etc. (see e.g. [10]). For instance, the unique fixed point of the Fitzhugh-Nagumo equation can be shown to be attractive and stable.

This singularity analysis can be difficult to fulfill (and even more when cycles are also considered – see e.g. the results about the *Hilbert’s sixteenth problem*). No general method can be expected to be applicable to every situation. Nevertheless, there exist other techniques which help to build faithful CA sequences. First, more classical features of qualitative phase portrait analysis can be used like *attraction basins*, *funnels*, and *anti-funnels* (see e.g. [10]). One can also apply *index theory* (see in particular *cell-to-cell mapping theory* [9]) or *singular perturbation theory* (see e.g. [22, 14]). To ensure the preservation of some global quantities, e.g. the energy of the system, one can consider *conservative numerical schemes* (see e.g. [17]). Finally, *cell-to-cell mapping theory* includes extensions based on Markov chains [9] from which probabilistic CA can be derived.

Summing up, we have seen that DE and CA can be formally related in many respects. Thus, there are cases where DE can be thought of as abstract reference objects to obtain faithful CA sequences, that is, descriptions that include qualitative as well as quantitative features. Qualitative descriptions can be adjusted and compared to quantitative solutions, and DE are used to give insights and tools to produce meaningful CA. As a result, CA can be tuned, DE-based simulations can be optimized (by attempting to find minimal CA), and more generally the qualitiveness of a global model can be studied. As further investigations, other faithful CA sequences could be produced (for instance considering other excitatory systems [18, 9, 15]). One could also establish connections with *qualitative physics and reasoning* [12] – where quantitative and qualitative descriptions are often mixed –, or with *ultradiscretization methods* [21] – able to transform DE into integrable CA over integers. Coupling invariant regions of phase portraits could lead to new interesting CA behaviors.

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