

Continuum versus Discrete: A Physically Interpretable General Rule for Cellular Automata by Means of Modular Arithmetic

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Describing complex phenomena by means of cellular automata (CAs) has shown to be a very effective approach in pure and applied sciences. In fact, the number of published papers concerning this topic has tremendously increased over the last 20 years. Most of the applications use CAs to qualitatively describe the phenomena, which is surely a consequence of the way the automata rules are commonly defined. In this paper, a physical application of a general rule that describes each of Stephen Wolfram's CAs is discussed. The new representation is given in terms of the so-called iota-delta function. The latter function is further generalized in order to provide a general rule for not only Wolfram's but also to every CA rule that depends on the sum and products of the values of cells in the automaton mesh. By means of a parallel between the finite difference method and the iota-delta function, a straightforward physical interpretation of CAs is derived. Such an application regards advective-diffusive phenomena without a constant source. Finally, the relation between CAs and anomalous diffusion is briefly discussed.

1. Introduction

It is undeniable that science has evolved to such a stage that almost every situation in everyday life has been, in some way, addressed. This can be clearly seen when, for example, technological development is taken into account. Such development provided people with better conditions to improve and build the society as it is known today. Do not forget, on the other hand, that knowledge and technology are intimately related. The most up-to-date gadgets employ state-of-the-art

concepts from physics, mathematics, and other basic sciences. In this way, the need to keep researching in basic sciences is inherent to the development of the so-called applied sciences, such as engineering.

This rigid segregation of the production and application of knowledge started changing when the complexity of everyday problems increased. Basic and applied sciences had to strengthen their bonds in order to give satisfactory answers to the problems that appeared. The atomic theory especially played a major role in this need of joint work.

At one point, notable physicists such as Werner Heisenberg, Niels Bohr, Max Planck, Erwin Schrödinger, and Louis de Broglie noticed that, even if they correctly applied the established knowledge, no plausible answer would be found for their questions about atomic structure. It is worth asking whether the questions of some of the greatest minds of our era were misformulated, or whether the main issue was not how questions were formulated, but what kinds of answers were expected. Schrödinger [1] gave a straightforward explanation to this apparent “anomaly” in science, as shown in [2]:

“[...] If you envisage the development of physics in the last half-century, you get the impression that the discontinuous aspect of nature has been forced upon us very much against our will. We seemed to feel quite happy with the continuum. Max Planck was seriously frightened by the idea of a discontinuous exchange of energy [...] Twenty-five years later the inventors of wave mechanics indulged for some time in the fond hope that they have paved the way of return to a classical continuous description, but again the hope was deceptive. Nature herself seemed to reject continuous description [...] The observed facts appear to be repugnant to the classical ideal of continuous description in space and time. [...] So the facts of observation are irreconcilable with a continuous description in space and time [...]”

Also, Fritjof Capra [3] brilliantly stated in his book:

“[...] Every time the physicists asked nature a question in an atomic experiment, nature answered with a paradox, and the more they tried to clarify the situation, the sharper the paradoxes became. It took them a long time to accept the fact that these paradoxes belong to the intrinsic structure of atomic physics, and to realize that they arise whenever one attempts to describe atomic events in the traditional terms of physics. [...]”

Both these excerpts can be readily exemplified by one of the most remarkable and, in some ways, unintentional changes in scientific ideas: the quantization of energy by Planck. While studying the second law of thermodynamics, Planck and Ludwig Boltzmann had a se-

rious rivalry. The former, at first, did not believe that entropy would be statistically described, while the latter firmly defended such an interpretation [4].

In order to give a consistent explanation to the increase of entropy predicted by thermodynamics, Planck and his contemporaries deeply analyzed James Clerk Maxwell's laws since these relations were supposed to govern the microscopic oscillators that produced the heat radiation emitted by black bodies [4]. After some time, Planck believed he had justified the irreversibility, and thus the entropy change, by means of the lack of symmetry of Maxwell's equations. Boltzmann promptly showed that Planck was wrong, impelling the latter to seek another way to explain the second law of thermodynamics [4].

While studying the black body radiation emission problem, Planck came up with a theoretically justifiable formula that matched well with experimental results. Sir Rayleigh and Sir James Jeans, at about the same time, proposed an energy distribution based on classical mechanics, that is, continuum theory. The Rayleigh–Jeans law (R-JL) led to a classical physical misinterpretation: the ultraviolet catastrophe. Following R-JL, the production of energy was proportional to the inverse of the fourth power of the wave length; when ultraviolet radiation is considered, as the wave length decreases, the energy production tends to infinity, which is absurd [4].

At the end of the year 1900, Planck noticed that the equation he proposed was more than a lucky shot and, in order to give it solid theoretical basis, he had to adopt some of Boltzmann's probabilistic ideas. By doing that, for the first time the Boltzmann equation appeared. In short, the latter equation relates entropy to molecular disorder. In order to quantify molecular disorder, Planck had to establish a method to count the number of ways a given energy can be distributed among a set of oscillators. The creation of the concept of quanta, discrete elements with finite portions of energy, was the answer to his questions [4].

The determinant issue while asking effective questions of nature is the dichotomy: continuum versus discrete. The continuity ideas date back to ancient times and seem to have found in Parmenides and Aristotle [5] their first defenders. By the modern age, Isaac Newton and Gottfried Leibniz established one of the pillars of the continuity principle: differential and integral calculus. Everything that is currently described by means of differential equations has the continuity principle as its background. Such a relation follows from the intrinsic linkage between differentiability and continuity of functions, leading to the “continuity” of the phenomena described. Scientists were so amazed by differential calculus that Bernhard Riemann once said [2]:

“[...] As is well known, physics became a science only after the invention of differential calculus. It was after realizing that natural phenomena are continuous that attempts to construct abstract models were successful. [...] True basic laws can only hold in the small and must be formulated as partial differential equations. Their integration provides the laws for extended parts of time and space. [...]”

By now, a very important remark has to be taken into consideration: continuity, in fact, provided mankind with an outstanding development. As stated, the field could not have come this far without continuity and its models. The purpose of this paper is not to depreciate the continuum ideas, but to propose a better approximation of nature's behavior since nature itself, in Schrödinger's words, seems “to reject continuous description.”

Riemann, maybe dazzled by the tremendous success arising from the application of differential equations in science, made a few statements which were, in some ways, trifling. As noticed by Lev Goldfarb [2], the assumption that natural phenomena were continuous seems to be postulated rather than noticed. An important question is whether the integration referred to by Riemann always applies. These questions have found their answers in the current scientific community: the growing usage of numerical methods in which finite elements or differences are taken into account shows that, once again, what was once thought to be continuous must be treated in a discrete way.

The basic idea behind the finite element method is mesh discretization of some continuous domain into a set of discrete sub-domains. The finite differences method, on the other hand, transforms differential equations into difference equations, the latter being a discrete “approximation” of the former.

If nature is shown to behave discretely, and the way to solve the governing equations of the established continuum theory is found to be by discrete differences and finite elements, it seems the scientific community keeps doubling its work.

It is remarkable how continuous models fit to circular, rectangular, square, and, in general, well-defined geometries. But, as the visionary Benoit Mandelbrot said [6]:

“[...] Clouds are not spheres, mountains are not cones, coastlines are not circles, and bark is not smooth, nor does lightning travel in a straight line. [...]”

Put in another way, the continuous domain works well when idealized problems are considered, but only discrete methods can answer complex problems. Complex, on the other hand, does not mean difficult or unsolvable. Complexity is inherent to nature. Wolfram, in his paradigm-shifting book *A New Kind of Science*, clearly showed that

simple rules—also referred to by Wolfram as programs—can generate complexity and intricate patterns [7].

At first, by means of a simple binary language, Wolfram proposed a class of computational experiments over a net of cells. The values of three cells determine how a fourth cell would be. Since each cell can have two possible states, there are eight possible trios. Each trio can result in two other values for the fourth cell, thus, there are 28 possibilities. Taking advantage of the binary scenario, Wolfram created the 0–255 classification, in which each combination receives a number from 0 to 255. This will be further explained in this paper.

The generalization from binary to ternary was immediate and Wolfram also presented it in his book. A concern shown by Wolfram was whether a general simple rule that would govern time, space, and energy in a given scale existed or not. In order to address this issue, the present paper shows that Wolfram's cellular automata (CAs) can be expressed by a single rule applied to the whole cellular net. It is then conjectured that every CA can be represented by a generalization of the referred rule. Also, by means of a parallel between the new general rule hereby defined and the finite difference method, it is possible for the first time to quantitatively describe CAs and the phenomena modeled by the latter.

2. Investigating Rules 0–255 of Wolfram's Cellular Automata

In the second chapter of *A New Kind of Science* [7], a simple yet tricky question is asked: “How do simple programs behave?” For sure, answering such a question is extremely difficult if it is attempted based merely on standard science. Prior to being able to predict the outcome, feeling, observing, and interacting are required. Computers provided mankind with the possibility to make contact with multiple realities, allowing the observation of the interaction between multiple phenomena at the same time.

In this way, Wolfram [7] shows that using computers to answer the previous question is not just a good way to address the issue, but the only method that can bring reliable results. Experimental computation led to the establishment of CAs, part of the basis of this new kind of science.

Start with the simplest CA available in [7]. In short, the classical definition is [7]:

“The cellular automaton consists of a line of cells, each colored black or white. At every step there is then a definite rule that determines the colour of a given cell from the colour of that cell and its immediate left and right neighbors on the step before.”

This excerpt can be better visualized by considering Figure 1.

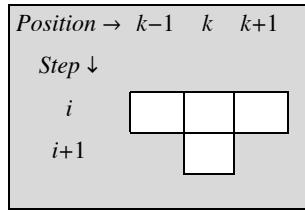


Figure 1. CA mesh.

As stated by Wolfram, three cells from the last step must be taken into account in order to define the color (or, as it is commonly described, the binary value 1 or 0) of a cell in the next step. In other words, the value of a given cell is given as a function of the values of three other cells. In order to give a mathematical description of this relation, consider the following representation:

$$C_k^{i+1} = f[C_{k-1}^i, C_k^i, C_{k+1}^i] \quad (1)$$

in which it is considered that the CA mesh is made of cells C , hereby indexed in space by the subscript k , and time by the superscript i , as in C_k^i . Since there are only two possible values for the cells, either 1 (black) or 0 (white), there are 2^3 possible combinations or trios, as seen in Figure 2.

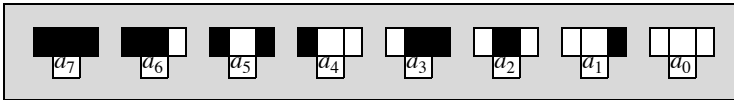


Figure 2. The eight possible trios.

Each value a_j , $j = 0, 1, \dots, 7$, is equivalent to 1 or 0; this way, a total of 2^8 possible rules are determined by the simple procedure we have described. Wolfram established a naming criteria for all the 256 possible trio combinations known as the 0–255 classification [7]. The rule is straightforward and relates the decomposition of the rule number in base 2 to the values of the coefficients a_j . For example, rule 30 has the following factorization:

$$30 = 0.2^7 + 0.2^6 + 0.2^5 + 1.2^4 + 1.2^3 + 1.2^2 + 1.2^1 + 0.2^0. \quad (2)$$

The coefficients a_j are the numbers that multiply 2^j in the factorization process. The set of trios that generate rule 30 are described in Figure 3.

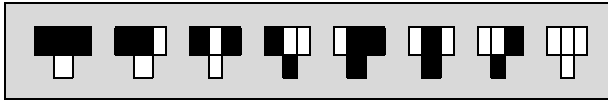


Figure 3. Rule 30.

In order to produce a compact notation, define the rule number function (RNF) as

$$\text{RNF}(a_0, a_1, a_2, a_3, a_4, a_5, a_6, a_7) = \sum_{j=0}^7 a_j 2^j. \tag{3}$$

The RNF provides the rule number given the values of the coefficients $a_j, j = 0, 1, \dots, 7$. This way, the logic is inverse: the function inputs are the coefficients and not the rule number. The latter is, on the other hand, the output of the transformation. The RNF can be generalized to a base b and a combination of n cells in the previous step as

$$\text{RNF}(v_0, v_1, v_2, \dots, v_{b^n-1}; b) = \sum_{j=0}^{b^n-1} v_j b^j; \tag{4}$$

$$0 \leq \text{RNF} \leq b^{b^n-1} - 1.$$

Given this brief introduction to CAs, consider another interesting rule: rule 90. Its trio representation is given in Figure 4.

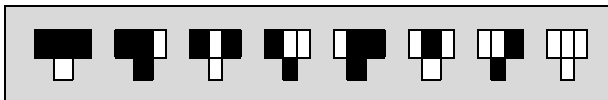


Figure 4. Rule 90.

In [7], the following relation was given to describe the behavior of rule 90:

$$C_k^{i+1} = \text{mod}[C_{k-1}^i + C_{k+1}^i, 2] \tag{5}$$

where $\text{mod}[o, p]$ denotes the modulus operator, which gives the rest of the division of o by p if o is greater than p or o itself, otherwise. In general, p is called the congruence modulus.

An interesting characteristic of equation (5) is its simplicity. Instead of needing eight different rules, as shown in Figure 4, just one rule can be applied to the whole net in order to get the desired pattern. Us-

ing the notation introduced in equation (1), Figure 4 gives

$$C_k^{i+1} = \begin{cases} 0, & \text{if } [C_{k-1}^i, C_k^i, C_{k+1}^i] = [1, 1, 1] \\ 1, & \text{if } [C_{k-1}^i, C_k^i, C_{k+1}^i] = [1, 1, 0] \\ 0, & \text{if } [C_{k-1}^i, C_k^i, C_{k+1}^i] = [1, 0, 1] \\ 1, & \text{if } [C_{k-1}^i, C_k^i, C_{k+1}^i] = [1, 0, 0] \\ 1, & \text{if } [C_{k-1}^i, C_k^i, C_{k+1}^i] = [0, 1, 1] \\ 0, & \text{if } [C_{k-1}^i, C_k^i, C_{k+1}^i] = [0, 1, 0] \\ 1, & \text{if } [C_{k-1}^i, C_k^i, C_{k+1}^i] = [0, 0, 1] \\ 0, & \text{if } [C_{k-1}^i, C_k^i, C_{k+1}^i] = [0, 0, 0]. \end{cases} \quad (6)$$

In order to provide simple representations for every elementary CA (ECA) as in equation (5), the definition of a new function, the iota-delta function, has been discussed in [8]. Section 3 shows a few definitions concerning this function.

3. The Iota-Delta Function

In order to represent every binary automaton, the iota-delta function has been defined in [8] as follows:

$$\begin{aligned} \iota\delta_n^m[x] &= \\ & \text{mod}[\text{mod}[\dots\text{mod}[\text{mod}[x, p_m], p_{m-1}], \dots, p_j], n], \quad (7) \\ m &\geq j; m, n \in \mathbb{Z}_+; x \in \mathbb{C}; j = \pi[n] + 1; \end{aligned}$$

in which m and n are parameters of the iota-delta function, p_m is the m^{th} prime number, and $\pi[n]$ stands for the prime counting function that gives the number of primes less than or equal to n . It is considered that $p_1 = 2$. The value of n determines how many states the automata generated have. Thus, for a binary automaton, $n = 2$, for ternary ones, $n = 3$, for quaternary ones, $n = 4$, and so on. Also, the iota-delta function is taken to be non-negative and $\max[\iota\delta_n^m[x]] \rightarrow n$ when $x \in \mathbb{R}$. A *Mathematica* code that readily implements equation (7) is [8]:

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iotaldelta[m_, n_, x_] := Mod[Fold[Mod[x, Table[Prime[m-j],
{j, 0, m-1-PrimePi[n]}]], n]

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It has been proposed in [8] that every ECA is represented by means of the general formulation

$$C_k^{i+1} = \iota\delta_n^m [\alpha_1 C_{k-1}^i + \alpha_2 C_k^i + \alpha_3 C_{k+1}^i + \alpha_4]. \quad (8)$$

The usage of equation (8) is fully justified by means of equation (1). Based on equation (8) and the cyclic property of the modular operator, the number of tuples $\{\alpha_1, \alpha_2, \alpha_3, \alpha_4\}$ allowed by means of the iota-delta function representation in equation (8) is p_m^4 , as the possible coefficients are $\alpha_j = \{r \mid r \leq p_m - 1; r \in \mathbb{Z}_+\}; j = 1, 2, 3, 4$.

In order to represent every binary CA in the simplest way possible, in [8] it has been shown that the smallest value of m is $m = 5$. This corresponds to the case where the iota-delta function represents $\text{mod}[\text{mod}[\text{mod}[\text{mod}[x, 11], 7], 5], 3], 2]$.

Given these few definitions of the iota-delta function, we proceed to its generalization in Section 4.

4. The Capital Iota-Delta Function

Since the most basic operations are addition, subtraction, multiplication, and division, it is expected that CAs can be described by means of such operations. This way, instead of considering the linear combination of cells, the situation in which products are also allowed must be considered. Both subtraction and division follow from addition and multiplication; this way, let the combination of powers, sums, and products of cells be taken into account. The capital iota-delta function can be defined as

$$\gamma_\omega I \Delta_n^m \left[C_k^i \left| \begin{matrix} (\beta_1, \mu_1), (\beta_2, \mu_2), \dots, (\beta_\omega, \mu_\omega) \\ [[u_1, u_2, \dots, u_\omega, \alpha_{u_1, u_2, \dots, u_\omega}]] \end{matrix} \right. \right] = \tag{9}$$

$$\omega \delta_n^m \left[\sum_{\lambda=0}^{\lambda} \left(\sum_{u_1+u_2+\dots+u_\omega=\lambda} \alpha_{u_1, u_2, \dots, u_\omega} \prod_{1 \leq c \leq \omega} (C_{k+\beta_c}^{i+\mu_c})^{u_c} \right) \right]$$

in which the following occur.

1. The second summation is taken over all combinations of non-negative integer indexes u_1 through u_ω such that the sum of all u_j is λ .
2. ω is the number of terms that are being combined. In other words, it represents how many cells the value of another given cell depends on. In equation (8), for example, $\omega = 3$ since the value of C_k^{i+1} depends on the value of three other cells, namely C_{k-1}^i , C_k^i , and C_{k+1}^i .
3. γ is the greatest power of any combined term. In equation (8), $\gamma = 1$ since there are no terms on the right-hand side that are raised to powers greater than one.
4. m and n are the parameters of the iota-delta function.

5. The pairs (β_c, μ_c) , $c = 1, \dots, \omega$ are functional parameters that locate the combined terms with respect to C_k^i . For example, for C_{k-1}^i , the pair is $(-1, 0)$.
6. $\alpha_{u_1, u_2, \dots, u_\omega}$ are the coefficients of the final terms for each set of values $u_1, u_2, \dots, u_\omega$. In fact, there is a total of $(\gamma + \omega)! / \gamma! \omega!$ of such coefficients. Besides, their values are $\alpha_{u_1, u_2, \dots, u_\omega} = \{r \mid r \leq p_m - 1; r \in \mathbb{Z}_+\}$. The notation $[[.]]$ stands for a matrix $(\gamma + \omega)! / \gamma! \omega!$ by $\omega + 1$ whose lines are correspondent to each set of values $u_1, u_2, \dots, u_\omega, \alpha_{u_1, u_2, \dots, u_\omega}$. In equation (8), the corresponding lines are $(0, 0, 0, \alpha_{0,0,0} = \alpha_4)$, $(1, 0, 0, \alpha_{1,0,0} = \alpha_1)$, $(0, 1, 0, \alpha_{0,1,0} = \alpha_2)$, and $(0, 0, 1, \alpha_{0,0,1} = \alpha_3)$. Based on the capital and the ordinary iota-delta functions, the general equation that represents every binary CA is given as

$$C_k^{i+1} = \frac{1}{3} I \Delta_2^5 \left[C_k^i \left[\begin{array}{c} (-1, 0), (0, 0), (1, 0) \\ \left[\begin{array}{c} \left[\begin{array}{c} 0 \ 0 \ 0 \ \alpha_{0,0,0} \\ 1 \ 0 \ 0 \ \alpha_{1,0,0} \\ 0 \ 1 \ 0 \ \alpha_{0,1,0} \\ 0 \ 0 \ 1 \ \alpha_{0,0,1} \end{array} \right] \end{array} \right] \right] \right] = \tag{10}$$

$$i \delta_n^m [\alpha_{0,0,0} + \alpha_{1,0,0} C_{k-1}^i + \alpha_{0,1,0} C_k^i + \alpha_{0,0,1} C_{k+1}^i].$$

An interesting special case of the capital iota-delta function is when $\alpha_{u_1, u_2, \dots, u_\omega} = \gamma! / (u_1! u_2! \dots! u_\omega!)$. This way, equation (9) reduces to

$$\gamma I \Delta_n^m \left[C_k^i \left[\begin{array}{c} (\beta_1, \mu_1), (\beta_2, \mu_2), \dots, (\beta_\omega, \mu_\omega) \\ \left[\begin{array}{c} u_1, u_2, \dots, u_\omega, \frac{\gamma!}{u_1! u_2! \dots! u_\omega!} \end{array} \right] \right] \right] = \tag{11}$$

$$i \delta_n^m \left[\frac{\sum_{c=1}^{\omega} (C_{k+\beta_c}^{i+\mu_c})^{\gamma+1} - 1}{\sum_{c=1}^{\omega} C_{k+\beta_c}^{i+\mu_c} - 1} \right].$$

In order to prove equation (11), consider the multinomial theorem [9]:

$$(x_1 + x_2 + \dots + x_\omega)^\lambda = \sum_{u_1+u_2+\dots+u_\omega=\lambda} \frac{\gamma!}{u_1! u_2! \dots! u_\omega!} \prod_{1 \leq c \leq \omega} (x_c)^{u_c}. \tag{12}$$

Let $x_c = C_{k+\beta_c}^{i+\mu_c}$, $c = 1, \dots, \omega$. This way, when $\alpha_{u_1, u_2, \dots, u_\omega} = \gamma! / (u_1! u_2! \dots! u_\omega!)$, both equations (9) and (12) provide

$$\begin{aligned} \gamma I \Delta_n^m \left[C_k^i \left[\left[\left[u_1, u_2, \dots, u_\omega, \frac{\gamma!}{u_1! u_2! \dots! u_\omega!} \right] \right] \right] \right] = \\ \iota \delta_n^m \left[\sum_{\lambda=0}^{\gamma} \left(\sum_{c=1}^{\omega} C_{k+\beta_c}^{i+\mu_c} \right)^\lambda \right] = \iota \delta_n^m \left[\frac{\sum_{c=1}^{\omega} \left(C_{k+\beta_c}^{i+\mu_c} \right)^{\gamma+1} - 1}{\sum_{c=1}^{\omega} C_{k+\beta_c}^{i+\mu_c} - 1} \right]. \end{aligned} \quad (13)$$

5. Quantitative Interpretation of Cellular Automata by Means of the Iota-Delta Function

In Section 4 it has been demonstrated that every 0–255 CA can be represented in terms of the iota-delta function as equation (10). In this section, a quantitative interpretation of this relation is deduced by comparing equation (10) to the finite difference method (FDM).

As widely known, FDM is a numerical method that turns differential equations into difference equations, making possible the solution of the former by solving a system of the latter. The methodology to be presented is applicable to every partial differential equation (PDE); on the other hand, in order to better explain the procedure, the advective-dispersive equation that describes, for example, the solute flow in a porous medium is taken into account. This way, let the equation that describes the concentration $c(x, t)$ of a given solute flowing in a porous medium as [10]

$$\frac{\partial c}{\partial t} = D_x \frac{\partial^2 c}{\partial x^2} - v_x \frac{\partial c}{\partial x} \quad (14)$$

in which $D_x [L^2/T]$ is the hydrodynamic dispersivity of the medium and $v_x [L/T]$ is the mean velocity of the interstitial fluid.

The reader is probably familiar with the concepts behind FDM, so basic definitions will be omitted. The latter can be further investigated in [11]. Use the forward difference in space and time for the first-order derivative. Also, the central difference for the second-order derivative in space shall be used. This way, by applying FDM to equation (14) considering a structured mesh whose lengths in space and

time are Δt and Δx , respectively, the latter equation turns to

$$\frac{c(x, t + \Delta t) - c(x, t)}{\Delta t} = D_x \frac{c(x + \Delta x, t) - 2c(x, t) + c(x - \Delta x, t)}{\Delta x^2} - v_x \frac{c(x + \Delta x, t) - c(x, t)}{\Delta x}. \quad (15)$$

In order to simplify notation and also clarify the link between FDM and CAs, let k be the position x in space and i the position t in time. It is clear that based on the mesh lengths described, the position $k + 1$ is equivalent to $x + \Delta x$ in the “real” space mesh and the position $i + 1$ is equivalent to $t + \Delta t$ in the “real” time mesh. Also, let the following substitutions take place:

$$N = \frac{D_x \Delta t}{\Delta x^2} \quad (16)$$

$$C_r = \frac{v_x \Delta t}{\Delta x} \quad (17)$$

in which N and C_r are the Neumann and Courant numbers, respectively. This way, equation (15) turns to

$$c_k^{i+1} = N c_{k-1}^i + (1 - 2N + C_r) c_k^i + (N - C_r) c_{k+1}^i. \quad (18)$$

It has been shown in [12] that the FDM scheme used in equation (18) is stable if

$$2N - C_r \leq 1. \quad (19)$$

The similarity between equations (8) and (18) is remarkable. The main question is how to directly relate one to the other. An immediate alternative is linear scaling of the iota-delta function in order to obtain equation (18). This way, consider a non-null scaling constant S multiplied to the right-hand side of equation (8). When $S = 1$, equation (8) is recovered. The new rule takes the form

$$C_k^{i+1} = S i \delta_n^m [\alpha_{0,0,0} + \alpha_{1,0,0} C_{k-1}^i + \alpha_{0,1,0} C_k^i + \alpha_{0,0,1} C_{k+1}^i]. \quad (20)$$

Consider the evolution of equation (20) for a unitary initial condition presented in Figure 5. Note that the evolution is given from left to right instead of the traditional up-down convention.

0	$S \iota \delta_2^5[\alpha_{0,0,0}]$	$S \iota \delta_2^5[\alpha_{0,0,0} + S \alpha_{0,1,0} \iota \delta_2^5[\alpha_{0,0,0}] + S \alpha_{1,0,0} \iota \delta_2^5[\alpha_{0,0,0}] + S \alpha_{0,0,1} \iota \delta_2^5[\alpha_{0,0,0} + \alpha_{0,0,1}]]$
0	$S \iota \delta_2^5[\alpha_{0,0,0} + \alpha_{0,0,1}]$	$S \iota \delta_2^5[\alpha_{0,0,0} + S \alpha_{1,0,0} \iota \delta_2^5[\alpha_{0,0,0}] + S \alpha_{0,1,0} \iota \delta_2^5[\alpha_{0,0,0} + \alpha_{0,0,1}] + S \alpha_{0,0,1} \iota \delta_2^5[\alpha_{0,0,0} + \alpha_{0,0,1}]]$
1	$S \iota \delta_2^5[\alpha_{0,0,0} + \alpha_{0,1,0}]$	$S \iota \delta_2^5[\alpha_{0,0,0} + S \alpha_{1,0,0} \iota \delta_2^5[\alpha_{0,0,0} + \alpha_{0,0,1}] + S \alpha_{0,1,0} \iota \delta_2^5[\alpha_{0,0,0} + \alpha_{0,1,0}] + S \alpha_{0,0,1} \iota \delta_2^5[\alpha_{0,0,0} + \alpha_{1,0,0}]]$
0	$S \iota \delta_2^5[\alpha_{0,0,0} + \alpha_{1,0,0}]$	$S \iota \delta_2^5[\alpha_{0,0,0} + S \alpha_{0,0,1} \iota \delta_2^5[\alpha_{0,0,0}] + S \alpha_{1,0,0} \iota \delta_2^5[\alpha_{0,0,0} + \alpha_{0,1,0}] + S \alpha_{0,1,0} \iota \delta_2^5[\alpha_{0,0,0} + \alpha_{1,0,0}]]$
0	$S \iota \delta_2^5[\alpha_{0,0,0}]$	$S \iota \delta_2^5[\alpha_{0,0,0} + S \alpha_{0,0,1} \iota \delta_2^5[\alpha_{0,0,0}] + S \alpha_{0,1,0} \iota \delta_2^5[\alpha_{0,0,0}] + S \alpha_{1,0,0} \iota \delta_2^5[\alpha_{0,0,0} + \alpha_{1,0,0}]]$

Figure 5. Evolution of equation (20).

In order to determine which is the value of S , compare the evolution of equation (20) to the evolution of the FDM scheme in equation (18). Thus, consider the evolution of the FDM scheme as in Figure 6.

0	0	$(-Cr + N)^2$
0	$-Cr + N$	$2(1 + Cr - 2N)(-Cr + N)$
1	$1 + Cr - 2N$	$(1 + Cr - 2N)^2 + 2N(-Cr + N)$
0	N	$2(1 + Cr - 2N)N$
0	0	N^2

Figure 6. Evolution of equation (18).

First and foremost, in order to be able to compare the values of both FDM and CA schemes, it is important to notice that the FDM scheme adopted depends only on a linear combination of the values of the variable of interest in a previous step. This way, it is possible to set $\alpha_{0,0,0} = 0$.

In order to turn the values concerning the CA approach independent of the ι - δ function, the argument of the ι - δ function in equation (20) has to be less than 2. This comes from the definition of the modular operator in the case of binary automata. Specifically,

if the maximum of the argument of the iota-delta function is less than 2, every other argument will also be. Consider the inequality

$$\alpha_{1,0,0} C_{k-1}^i + \alpha_{0,1,0} C_k^i + \alpha_{0,0,1} C_{k+1}^i \leq S(\alpha_{1,0,0} + \alpha_{0,1,0} + \alpha_{0,0,1}). \quad (21)$$

In order to find the value of S , notice that the coefficients of the FDM scheme in each line always add up to 1. This is due to the conservative behavior of the problem considered. Consider that the first line of the CA evolution adds up to Ω . Thus,

$$S(\iota\delta_n^m[\alpha_{1,0,0}] + \iota\delta_n^m[\alpha_{0,1,0}] + \iota\delta_n^m[\alpha_{0,0,1}]) = \Omega. \quad (22)$$

Assuming that S exists such that each line of the CA will add up to the same Ω , in order to normalize the lines obtained from the CA approach each line must be divided by such a constant. Finally, from equation (22) and Figures 5 and 6, it is possible to obtain the following system of equations:

$$\begin{aligned} N - C_r &= \frac{S \iota\delta_n^m[\alpha_{0,0,1}]}{\Omega} = \frac{\iota\delta_n^m[\alpha_{0,0,1}]}{\iota\delta_n^m[\alpha_{1,0,0}] + \iota\delta_n^m[\alpha_{0,1,0}] + \iota\delta_n^m[\alpha_{0,0,1}]} \\ N &= \frac{S \iota\delta_n^m[\alpha_{1,0,0}]}{\Omega} = \frac{\iota\delta_n^m[\alpha_{1,0,0}]}{\iota\delta_n^m[\alpha_{1,0,0}] + \iota\delta_n^m[\alpha_{0,1,0}] + \iota\delta_n^m[\alpha_{0,0,1}]} \end{aligned} \quad (23)$$

which can be readily solved as

$$\begin{aligned} C_r &= \frac{\iota\delta_n^m[\alpha_{1,0,0}] - \iota\delta_n^m[\alpha_{0,0,1}]}{\iota\delta_n^m[\alpha_{1,0,0}] + \iota\delta_n^m[\alpha_{0,1,0}] + \iota\delta_n^m[\alpha_{0,0,1}]} \\ N &= \frac{\iota\delta_n^m[\alpha_{1,0,0}]}{\iota\delta_n^m[\alpha_{1,0,0}] + \iota\delta_n^m[\alpha_{0,1,0}] + \iota\delta_n^m[\alpha_{0,0,1}]} \end{aligned} \quad (24)$$

By means of equation (24) and the stability conditions in equation (19), it is possible to analyze the stability of CA schemes representing advective-dispersive phenomena. This way,

$$2N - C_r = \frac{\iota\delta_n^m[\alpha_{1,0,0}] + \iota\delta_n^m[\alpha_{0,0,1}]}{\iota\delta_n^m[\alpha_{1,0,0}] + \iota\delta_n^m[\alpha_{0,1,0}] + \iota\delta_n^m[\alpha_{0,0,1}]} \leq 1. \quad (25)$$

Equation (25) shows that CA schemes representing advective-dispersive phenomena are always stable, as expected from CA theory.

Finally, if the right-hand side of equation (21) must be less than 2, the left-hand side also must be. It can be shown that only when the right-hand side of equation (21) is equal to 1 is the condition that each line of the CA adds up to Ω satisfied. The latter proof consists of

equating the sum of the terms in the second and third columns in Figure 5. For simplicity, the proof is omitted. This way, S can be readily obtained as

$$S = \frac{1}{\alpha_{1,0,0} + \alpha_{0,1,0} + \alpha_{0,0,1}}. \quad (26)$$

By means of these formulas, CA schemes prove their value as convergent explicit methods to describe systems once only described by means of PDEs. Also, it is interesting to explore the diffusive case, when the Courant number is 0. In this case, note that FDM schemes demand the coefficients in equation (18) be symmetric, that is, both the first and last are equal to N . On the other hand, the CA scheme only requires that the iota-delta of the coefficients to be symmetric. This way, a very interesting feature of the CA scheme shows up: the possibility of dealing with normal and anomalous diffusion by means of a single formulation. This will be better explained in Section 6.

6. Normal Diffusion and Anomalous Diffusion by Means of Cellular Automata

As stated in Section 5, for an FDM scheme, normal diffusion is obtained when the coefficients are symmetric with respect to the initial condition space row. On the other hand, when the iota-delta functions of the coefficients that define the automaton rule are symmetric with respect to the initial condition space row, not only normal diffusion but also anomalous behavior is easily seen. At first, a question that demands an answer is whether the CA approach for describing diffusive problems gives the same answer as the FDM scheme. In order to address this issue, we must take into account two conditions.

6.1 Condition 1

Are the coefficients of the CA methodology symmetric with respect to the initial condition line? In order to address this first condition, consider the coefficients in the first and last lines of the last column in Figure 5. Based on this observation, in order to have symmetry with respect to the initial condition line, we must have

$$\frac{S \iota \delta_n^m [\alpha_{1,0,0} S \iota \delta_n^m [\alpha_{1,0,0}]]}{\Omega} = \frac{S \iota \delta_n^m [\alpha_{0,0,1} S \iota \delta_n^m [\alpha_{0,0,1}]]}{\Omega}. \quad (27)$$

In the diffusive case, from equation (24), $\iota \delta_n^m [\alpha_{1,0,0}] = \iota \delta_n^m [\alpha_{0,0,1}]$. Thus, both iota-delta functions are either 0 or 1, following the binary characterization. When they are 0, it is clear that equation (27) is

fully satisfied. On the other hand, when they are both 1, the argument of the outer iota-delta function becomes less than 2 since S is the inverse of the sum of the three coefficients, which finally takes the argument out of the iota-delta function and leads to $\alpha_{1,0,0} = \alpha_{0,0,1}$. It has been proved that in order to obtain symmetric diffusion with respect to the initial condition position, both the coefficients and their iota-delta functions have to be equal. Now we must investigate the second and most important condition.

6.2 Condition 2

Are the outer coefficients of the CA methodology related to the ones in the previous step? If yes, what is the relation?

It is clear from Figure 6 that the outer coefficients of the FDM scheme are related to the ones in the previous steps by a power function. In order to better develop this part of the paper, Neumann numbers will also be indexed in space and time; thus, the FDM shows that, for a diffusive case,

$$N_{-i}^i = (N_{-1}^1)^i; \quad N_i^i = (N_1^1)^i \quad i \geq 1. \quad (28)$$

From equation (24), the corresponding Neumann numbers in the CA scheme are $N_{-1}^1 = N_1^1 = S/\Omega$. CA methodology provides, on the other hand,

$$N_{-i}^i = \frac{S \iota \delta_n^m [\alpha_{0,0,1} \Omega N_{-i+1}^{i-1}]}{\Omega}; \quad (29)$$

$$N_i^i = \frac{S \iota \delta_n^m [\alpha_{1,0,0} \Omega N_{i-1}^{i-1}]}{\Omega} \quad i \geq 2.$$

Equation (29) easily implies

$$N_{-i}^i = \frac{S^i (\alpha_{0,0,1})^{i-1}}{\Omega}; \quad N_i^i = \frac{S^i (\alpha_{1,0,0})^{i-1}}{\Omega} \quad i \geq 1. \quad (30)$$

There are three situations concerning equations (28) and (30).

6.2.1 Two-Sided Lighter-Tailed Anomalous Diffusion

Two-sided lighter-tailed anomalous diffusion occurs when

$$N_{-i}^i = \frac{S^i (\alpha_{0,0,1})^{i-1}}{\Omega} < \frac{S^i}{\Omega^i}; \quad (31)$$

$$N_i^i = \frac{S^i (\alpha_{1,0,0})^{i-1}}{\Omega} < \frac{S^i}{\Omega^i} \quad i \geq 1.$$

By lighter tailed, we consider the comparison with the standard diffusion hereby represented by the FDM approach. Note that equation (31) physically suggests that the last values of the CA scheme are lower than the ones of the FDM scheme, which implies a lighter-tailed distribution of concentrations in the former compared to the latter. From equation (31), we get

$$\begin{aligned} \alpha_{0,0,1} \iota \delta_n^m [\alpha_{0,1,0}] &< \alpha_{1,0,0} + \alpha_{0,1,0} - \alpha_{0,0,1}; \\ \alpha_{1,0,0} \iota \delta_n^m [\alpha_{0,1,0}] &< \alpha_{0,0,1} + \alpha_{0,1,0} - \alpha_{1,0,0}. \end{aligned} \tag{32}$$

Pay close attention to the fact that equation (32) gives the relation between the coefficients in order to be configured as a two-sided lighter-tailed anomalous diffusion. The one-sided case takes place when only one of the inequalities in equation (32) is satisfied. For the symmetric case, when $\alpha_{1,0,0} = \alpha_{0,0,1}$, equation (32) turns into

$$\alpha_{0,0,1} \iota \delta_n^m [\alpha_{0,1,0}] < \alpha_{0,1,0}; \quad \alpha_{1,0,0} \iota \delta_n^m [\alpha_{0,1,0}] < \alpha_{0,1,0}. \tag{33}$$

As an example, consider rule 150. Its capital iota-delta representation is

$$C_k^{i+1} = \frac{1}{3} I \Delta_2^5 \left[C_k^i \begin{array}{c} (-1, 0), (0, 0) (1, 0) \\ \left[\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 4 \\ 0 & 0 & 1 & 1 \end{array} \right] \end{array} \right]. \tag{34}$$

Also, equation (24) provides $N = 1/3$. For the rule in equation (34), both inequalities in equation (33) are satisfied, which characterizes a two-sided lighter-tailed concentration distribution, as can be seen in Figure 7 in which a corresponding FDM with $N = 1/3$ is

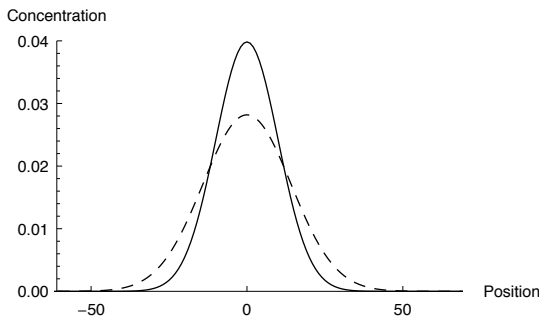


Figure 7. Comparison between the CA methodology for rule 150 (solid) and the corresponding FDM scheme (dashed) after 300 time steps.

also plotted. Since the relation between the discretized time and space and the real ones is $t = i \Delta t$ and to $x = k \Delta x$, respectively, the lengths of the mesh are just scale factors. In this way, Figure 7 has been plotted with the initial condition in the position $i = k = 0$ and the mesh lengths were taken as the unit.

By means of equations (28) and (30), it is clear that the Neumann number changes as the time steps evolve. In equation (16) the physical meaning of the Neumann number has been given, which implies verifying which physical parameter is changing over time. Considering that the mesh is not changing in time, from equations (16), (28), and (30) we find that the diffusivity of the medium for a symmetric two-sided lighter-tailed diffusion is given as

$$D_x = S \frac{\Delta x^2}{\Delta t} \frac{(\alpha_{0,0,1})^{(i-1)/i}}{\sqrt{i\Omega}}. \quad (35)$$

The discretization of the cellular net led to $t = i \Delta t$; thus equation (35) becomes

$$D_x = S \frac{\Delta x^2}{\Delta t} \frac{(\alpha_{0,0,1})^{(t-\Delta t)/t}}{\Omega(\Delta t)/t}; \quad t \geq \Delta t. \quad (36)$$

An amazing feature of equation (36) is the fact that the diffusivity varies following a power-law relation, which is the base of scaling properties in fractal structures. The comparison between the diffusivity of a CA and FDM schemes is given in Figure 8. The same considerations concerning the mesh lengths used to interpret Figure 7 are also applicable to Figure 8.

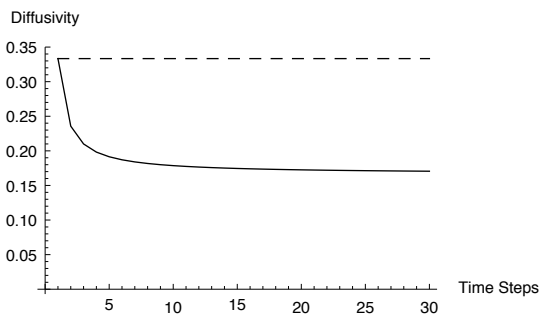


Figure 8. Comparison between the diffusivity of a CA methodology for rule 150 (solid) and the corresponding FDM scheme (dashed).

From equation (35), when i is big enough and by means of standard limit application rules, it is easy to get

$$D_x^{\text{steady}} = S \frac{\Delta x^2 \alpha_{0,0,1}}{\Delta t}. \quad (37)$$

Note that using the limit in equation (35) in which a given value is taken to tend to infinity does not invalidate the discreteness of the approach, since this type of limit only considers a large number of times steps, which is physically acceptable. The index steady has been added to the diffusivity D in order to show that this value is obtained for large times. It is very interesting to observe that even if the CA scheme has constant coefficients in its generating rule, a time-dependent behavior is seen for the diffusivity.

6.2.2 Two-Sided Light-Tailed Normal Diffusion

The two-sided light-tailed normal diffusion, or FDM approach, is the case when both the CA methodology and the FDM scheme give the same results. This way,

$$\begin{aligned} N_{-i}^i &= \frac{S^i (\alpha_{0,0,1})^{i-1}}{\Omega} = \frac{S^i}{\Omega^i}; \\ N_i^i &= \frac{S^i (\alpha_{1,0,0})^{i-1}}{\Omega} = \frac{S^i}{\Omega^i} \quad i \geq 1. \end{aligned} \quad (38)$$

Following an argument similar to the one employed in Section 6.2.1, the following hold for the case when CA and FDM give the same results:

$$\begin{aligned} \alpha_{0,0,1} \iota \delta_n^m [\alpha_{0,1,0}] &= \alpha_{1,0,0} + \alpha_{0,1,0} - \alpha_{0,0,1}; \\ \alpha_{1,0,0} \iota \delta_n^m [\alpha_{0,1,0}] &= \alpha_{0,0,1} + \alpha_{0,1,0} - \alpha_{1,0,0}. \end{aligned} \quad (39)$$

For the symmetric case,

$$\begin{aligned} \alpha_{0,0,1} \iota \delta_n^m [\alpha_{0,1,0}] &= \alpha_{0,1,0}; \\ \alpha_{1,0,0} \iota \delta_n^m [\alpha_{0,1,0}] &= \alpha_{0,1,0}. \end{aligned} \quad (40)$$

Also from equations (16) and (38), the diffusivity is given as

$$D_x = S \frac{\Delta x^2 \alpha_{0,0,1}}{\Delta t} \quad (41)$$

which is compatible with the normal diffusion situation in which the diffusivity is constant over time. Consider rule 22. Its capital iota-delta function representation can be readily identified as

$$C_k^{i+1} = \frac{1}{3} I \Delta_2^5 \left[C_k^i \begin{array}{c} (-1, 0), (0, 0) (1, 0) \\ \left[\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{array} \right] \end{array} \right] \tag{42}$$

which also gives $N = 1/3$. Even Neumann numbers of the corresponding FDM schemes are the same for rules 150 and 22; only the latter is the corresponding FDM method itself, since equations (38) through (40) are satisfied by the latter. There is no special physical meaning for the case in Section 6.2.2, thus no figures will be shown.

6.2.3 Two-Sided Heavier-Tailed Anomalous Diffusion

The two-sided heavier-tailed anomalous diffusion is now discussed.

The term heavier tailed is, as in Section 6.2.1, with respect to the ordinary FDM scheme. By means of an approach similar to that used in Sections 6.2.1 and 6.2.2, a two-sided heavier-tailed anomalous diffusion takes place when

$$N_{-i}^i = \frac{S^i(\alpha_{0,0,1})^{i-1}}{\Omega} > \frac{S^i}{\Omega^i};$$

$$N_i^i = \frac{S^i(\alpha_{1,0,0})^{i-1}}{\Omega} > \frac{S^i}{\Omega^i} \quad i \geq 1. \tag{43}$$

Also,

$$\alpha_{0,0,1} \iota \delta_n^m [\alpha_{0,1,0}] > \alpha_{1,0,0} + \alpha_{0,1,0} - \alpha_{0,0,1};$$

$$\alpha_{1,0,0} \iota \delta_n^m [\alpha_{0,1,0}] > \alpha_{0,0,1} + \alpha_{0,1,0} - \alpha_{1,0,0}. \tag{44}$$

For the symmetric case,

$$\alpha_{0,0,1} \iota \delta_n^m [\alpha_{0,1,0}] > \alpha_{0,1,0};$$

$$\alpha_{1,0,0} \iota \delta_n^m [\alpha_{0,1,0}] > \alpha_{0,1,0}. \tag{45}$$

Note that equations (35) through (37) are also valid for this case. As an example, take rule 54 and its capital iota-delta representation, which is

$$C_k^{i+1} = \frac{1}{3} I \Delta_2^5 \left[C_k^i \begin{array}{c} (-1, 0), (0, 0) (1, 0) \\ \left[\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 4 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 4 \end{array} \right] \end{array} \right] \quad (46)$$

which provides $N = 1/3$. Figures 9 and 10 show the behavior of rule 54 compared to the corresponding FDM scheme, based on the same premises used to investigate Figures 7 and 8.

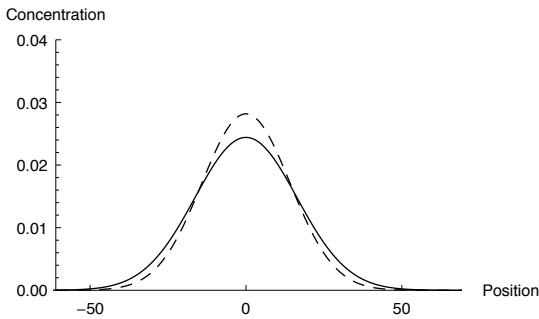


Figure 9. Comparison between the CA methodology for rule 54 (solid) and the corresponding FDM scheme (dashed) after 300 time steps.

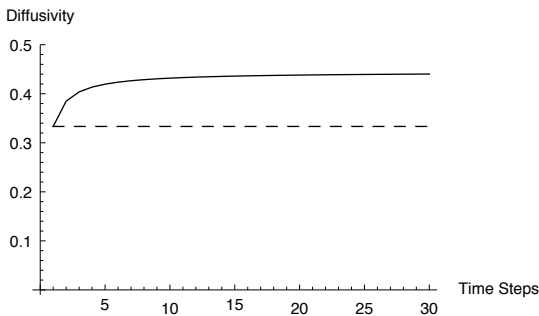


Figure 10. Comparison between the diffusivity of a CA methodology for rule 54 (solid) and the corresponding FDM scheme (dashed).

In the case where heavier-tailed behavior is seen, diffusivity grows in time, achieving its steady-state value given in equation (37).

An outstanding behavior can be seen by noticing that the steady-state diffusivity is the diffusivity of another FDM scheme with different parameters, as the comparison of equations (37) and (41) shows.

This is a physically justified behavior since after a long period of time, the differences between anomalous and normal diffusion tend to 0 as the concentration tends to be equally distributed all over the domain.

Another interesting behavior can be seen when asymmetric diffusive rules are taken into account. In order to investigate this behavior, consider, for example, rule 146. Its capital iota-delta representation is

$$C_k^{i+1} = \frac{1}{3} I \Delta_2^5 \left[C_k^i \begin{array}{c} (-1, 0), (0, 0), (1, 0) \\ \left[\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 2 \\ 0 & 0 & 1 & 1 \end{array} \right] \end{array} \right] \tag{47}$$

which provides $N = 0.5$. On the other hand, rule 26 has a capital iota-delta representation readily identified as

$$C_k^{i+1} = \frac{1}{3} I \Delta_2^5 \left[C_k^i \begin{array}{c} (-1, 0), (0, 0), (1, 0) \\ \left[\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 2 \\ 0 & 0 & 1 & 4 \end{array} \right] \end{array} \right] \tag{48}$$

which also gives $N = 0.5$. Even the Neumann numbers are the same and both CA schemes are representative of pure diffusion. The behavior described is radically different as can be seen in Figures 11 and 12.

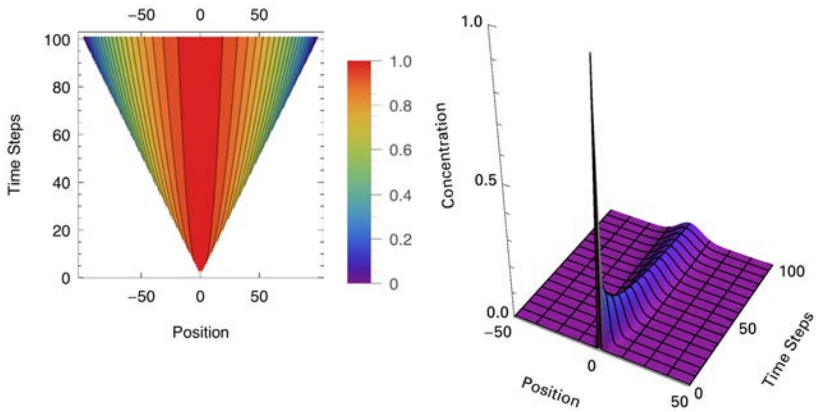


Figure 11. Log10 of the concentration (left) and evolution (right) for the ECA 146 scheme.

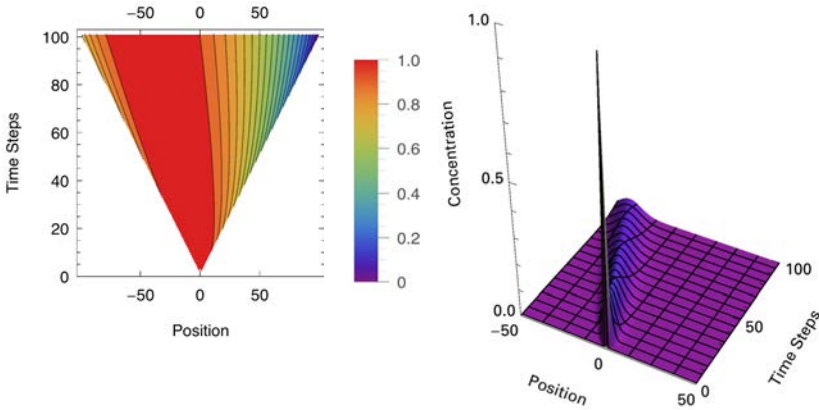


Figure 12. Log10 of the concentration (left) and evolution (right) for the ECA 26 scheme.

Figure 11 shows a symmetric diffusion while Figure 12 shows an asymmetric distribution whose peak is constantly moving. It is undeniable that anomalous diffusion takes place in the latter figure. This leads to a new understanding of how normal and anomalous diffusion are correlated. It can be said that normal diffusive processes are doubly symmetric while anomalous diffusion is only symmetric once. Correlating CAs and physical processes described by them to symmetry shows once more how valuable the latter is in science.

7. Conclusions

Nature seems to be discrete; notwithstanding, the current scientific society is still dominated by the continuum idea. In order to empower the discrete notion, scientists have to develop methods to quali-quantitatively describe nature's behavior taking into account the discreteness in the latter. Cellular automata (CAs) have shown to be an accurate description of some complex phenomena. In this paper, a general transformation that can be applied to the whole cellular net is discussed. By means of such a transformation, every binary, that is, 0–255 CAs are described.

In order to provide a compact version of the transformation developed, the iota-delta function has been used. The iota-delta function is further generalized in order to describe every CA. Such generalization is the capital iota-delta function, which is related to set partition and the multinomial theorem.

By means of a correlation between the iota-delta function and the finite difference method, 0–255 CAs could be described as advective-

dispersive processes. A new intuition has been brought up concerning normal and anomalous diffusion. It is worth noting that such an intuition could not have been deduced from partial differential equations (PDEs) and continuum theory since CA modeling of nature was fundamental in obtaining it. This paper intends to bring to discussion the iota-delta function and how the latter can be successfully applied to quantitatively describe CAs. Besides, the new intuition introduced seems to have interesting physical features that were not present in the previous definition of CAs. Also, some questions concerning CAs such as universality may be better analyzed by means of the iota-delta function.

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