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EDGE OF CHAOS IN REACTION-DIFFUSION CNN MODELS*

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In this paper different reaction-diffusion Cellular Nonlinear Networks (RD-CNN) models will be presented. Dynamics of Oregonator RD-CNN model will be studied. Local activity theory will be applied in order to determine the edge of chaos domain of the parameter set in which the model under consideration can exhibit complexity. Simulations and applications will be provided.

1. Introduction

Spatial and spatio-temporal patterns occur widely in physics, chemistry and biology. In many cases, they seem to be generated spontaneously. These phenomena have motivated a great deal of mathematical modelling and the analysis of the resultant systems has led to a greater understanding of the underlying mechanisms. Partial differential equations of diffusion type have long served as models for regulatory feedbacks and pattern formation in aggregates in living cells. In this work we proposed receptor-based models for pattern formation and regulation in multicellular biological systems. The systems describing our models are composed of both diffusion-type and ordinary differential equations. Such systems cause some difficulty, since both existence and behavior of the solutions are

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more difficult to establish. Many aspects of qualitative behavior have to be investigated numerically. For this purpose we apply the Cellular Nonlinear Networks (CNN) approach for studying such models.

We are witnessing a technical development in our fields where the sensing, computing, activating circuits and systems are becoming inherently connected; physically and theoretically, as well. Moreover, as a result of this, our notion about sensory computing, even about computing, is in a continuous transformation. Hence, we have to make a closer look about the fundamentals of computing. How, now, can we characterize a brain-like system? We might summarize the key properties as follows:

- Continuous time continuous (analog) valued signal arrays (flows)
- Several 2Dimensional strata of analog "processors" (neurons)
- Typically, mainly local, or sparse global (bus-like) interconnections
- Sensing and processing are integrated
- Vertical interconnections between a few strata of neuron "processors"
- Variable delays
- Spatial-temporal active waves
- Events are patterns in space and/or time

These features are already strongly modifying our view and practice in building complex electronic systems, including sensing, computing, activating and communicating devices and systems. This way of thinking, however, is supposing a completely different architecture, physical and algorithmic alike, and supposes tens of thousands or millions of parallel physical processing devices.

In developing a universal and canonical computing architecture, after having been decided the forms of data, we are tending to use the simplest possible building blocks, with the simplest possible interconnections, elementary instructions and programming constructs. Then we introduce algorithmic stored programmability to make it universal and practical. A most successful example is the digital computer, with a core universal machine on integers (Turing machine). What if we would make a brain-like computer with the properties shown above? The data are topographic (image) flows. In the simplest case, a pixel array with each pixel having a light intensity of gray values between black (say, +1) and white (say, -1) values. Color pictures are composed of several pictures with different color content. A special case is a binary mask. Now, let us construct a programmable topographic cellular sensory dynamics, as implementing the protagonist elementary instruction. The recipe is as follows:

- Take the simplest dynamical system, a cell (with input u , state x and output y)

- Take the simplest spatial grid for placing the cells with the simplest neighborhood relation (2D sheets)
- Introduce the simplest spatial interactions between dynamic cells, being programmable (called cloning template or gene, or simply template)
- Add cellular sensors.

CNN is simply an analogue dynamic processor array, made of cells, which contain linear capacitors, linear resistors, linear and nonlinear controlled sources. Let us consider a two-dimensional grid with 3×3 neighborhood system.

One of the key features of a CNN is that the individual cells are nonlinear dynamical systems, but that the coupling between them is linear. Roughly speaking, one could say that these arrays are nonlinear but have a linear spatial structure, which makes the use of techniques for their investigation common in engineering or physics attractive.

We will give the general definition of a CNN which follows the original one [2]:

Definition 1. *The CNN is a*

- a). 2-, 3-, or n - dimensional array of
- b). mainly identical dynamical systems, called cells, which satisfies two properties:
- c). most interactions are local within a finite radius r , and
- d). all state variables are continuous valued signals.

Definition 2. *An $M \times M$ cellular neural network is defined mathematically by four specifications:*

- 1). CNN cell dynamics;
- 2). CNN synaptic law which represents the interactions (spatial coupling) within the neighbor cells;
- 3). Boundary conditions;
- 4). Initial conditions.

In terms of Definition 2 we can present the dynamical systems describing CNN. For a general CNN whose cells are made of time-invariant circuit elements, each cell $C(ij)$ is characterized by its CNN cell dynamics :

$$(1) \quad \dot{x}_{ij} = -g(x_{ij}, u_{ij}, I_{ij}^s),$$

where $x_{ij} \in \mathbf{R}^m$, u_{ij} is usually a scalar. In most cases, the interactions (spatial coupling) with the neighbor cell $C(i+k, j+l)$ are specified by a CNN synaptic

law:

$$(2) \quad \begin{aligned} I_{ij}^s &= A_{ij,kl}x_{i+k,j+l} + \\ &+ \tilde{A}_{ij,kl} * f_{kl}(x_{ij}, x_{i+k,j+l}) + \\ &+ \tilde{B}_{ij,kl} * u_{i+k,j+l}(t). \end{aligned}$$

The first term $A_{ij,kl}x_{i+k,j+l}$ of (2) is simply a linear feedback of the states of the neighborhood nodes. The second term provides an arbitrary nonlinear coupling, and the third term accounts for the contributions from the external inputs of each neighbor cell that is located in the N_r neighborhood.

2. Reaction-diffusion CNN

It is known that some autonomous CNN represent an excellent approximation to nonlinear partial differential equations (PDEs). The intrinsic space distributed topology makes the CNN able to produce real-time solutions of nonlinear PDEs. Consider the following well-known PDE, generally referred to us in the literature as a reaction-diffusion equation:

$$\frac{\partial u}{\partial t} = f(u) + D\nabla^2 u,$$

where $u \in \mathbf{R}^N$, $f \in \mathbf{R}^N$, D is a matrix with the diffusion coefficients, and $\nabla^2 u$ is the Laplacian operator in \mathbf{R}^2 . There are several ways to approximate the Laplacian operator in discrete space by a CNN synaptic law with an appropriate A -template.

As a first example of CNN models we will consider the Fisher equation. Sixty years ago Fisher showed that the propagation of a mutant gene can be modeled by a nonlinear reaction-diffusion partial differential equation (PDE):

$$(3) \quad \frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} + f(u).$$

where $f(u) = qu(1 - u)$. This classic equation, also known as the ‘‘diffusional logistic’’ equation, has since been found to be useful in many other applications and has been widely studied. In chemical media the function $u(t, x)$ is the concentration of the reactant, D represents its diffusion coefficient, and the positive constant q specifies the rate of the chemical reaction. In media of other natures u, D, q can represent different quantities. In general, medium described by (3) is often refer to as a bistable medium, because it has two homogeneous stationary states, $u = 0$ and $u = 1$. Observe the case when $f(u) = u(u - 1)(u - E)$ in which

$f(u)$ has three zeros; namely, at $u = 0, E$ and 1 . This generalized model arises in many areas of ecology, including selection-migration models and other bistable population models. It is also found in a degenerate form of Nagumo's equation.

After rescaling time $t' = qt$ and space $x' = (q/D)^{1/2}x$, and dropping the prime, (3) in one-dimensional space becomes:

$$(4) \quad u_t = u_{xx} + u(1 - u).$$

As we mentioned, Fisher equation (4) can be presented by a reaction-diffusion autonomous CNN where the cells are a degenerate special case of Chua's oscillator [5]. We will map $u(x, t)$ into a CNN layer such that the state voltage of a CNN cell $x_{kl}(t)$ at a grid point (k, l) is associated with $u(kh, t)$, $h = \Delta x$. Therefore, an one-dimensional Laplacian template will be in the following form:

$$A_1 = (1, -2, 1),$$

and the CNN model in this case is:

$$(5) \quad \frac{du_k}{dt} = (u_{k-1} - 2u_k + u_{k+1}) + u_k(1 - u_k),$$

$k = 1, \dots, n$, $n = M.M$, where we have $M \times M$ cells.

In a two-dimensional isotropic medium Fisher's equation (3) in rescaled variables is:

$$(6) \quad u_t = u_{xx} + u_{yy} + u(1 - u).$$

The solution $u(x, y, t)$ of (6) is a continuous function of the time t and the space variables x, y . We shall approximate the function $u(x, y, t)$ by a set of functions $u_{jk}(t)$ which are defined as

$$u_{jk}(t) = u(jh_x, kh_y, t),$$

where h_x and h_y are the space intervals in the x and y coordinates. Then, two-dimensional discretized Laplacian A template will be in the following form:

$$A_2 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

The CNN model for two-dimensional Fisher's equation (6) will be [5]:

$$(7) \quad \frac{du_{jk}}{dt} = (u_{jk-1}(t) + u_{jk+1}(t) - 4u_{jk}(t) + u_{j-1k}(t) + u_{j+1k}(t)) \\ + u_{jk}(t)(1 - u_{jk}(t)) = (u_{jk-1}(t) + u_{jk+1}(t) - 4u_{jk}(t) \\ + u_{j-1k}(t)u_{j+1k}(t)) + n_{jk}(t),$$

$$1 \leq j \leq M, 1 \leq k \leq M.$$

Another most widely studied nonlinear reaction-diffusion partial differential equation (PDE) is the Brusselator equation, whose dimensionless equation is [5]:

$$(8) \quad \begin{aligned} \frac{\partial u}{\partial t} &= a - (b+1)u + u^2v + D_1 \nabla^2 u \\ \frac{\partial v}{\partial t} &= bu - u^2v + D_2 \nabla^2 v, \end{aligned}$$

where $\nabla^2 = \frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2}$ is a two-dimensional Laplacian operator in \mathbf{R}^2 , a, b are coefficients of the chemical reaction which give the concentration of initial substances, D_1, D_2 are diffusion coefficients. The Brusselator equation (8) is well known in chemical kinetics as an ideal system for studying the dissipative structures. In some sense this system behaves as harmonic oscillator.

Our CNN model for the Brusselator equation (8) with A_2 -template can be written in the following form:

$$(9) \quad \begin{aligned} u_{jk} &= a - (b+1)u_{jk} + u_{jk}^2 v_{jk} + D_1 [u_{j+1k} + \\ &\quad + u_{j-1k} + u_{jk+1} + u_{jk-1} - 4u_{jk}] \\ v_{jk} &= bu_{jk} - u_{jk}^2 v_{jk} + D_2 [v_{j+1k} + v_{j-1k} + v_{jk+1} + v_{jk-1} - 4v_{jk}], \end{aligned}$$

$$1 \leq j \leq M, 1 \leq k \leq M.$$

The other model we consider is a more general form of the Hodgkin-Huxley model for the propagation of the voltage pulse through a nerve axon which is referred to as the FitzHugh-Nagumo equation [5, 6]:

$$(10) \quad u_t - u_{xx} = u(u - \Theta)(1 - u) - b \int_0^t u(s, x) ds,$$

$0 < x, t < 1, 0 < \Theta < 1/2, b \geq 0$. The proposed equation (10) is nonlinear parabolic integro-differential equation, in which u_t is the first partial derivative of $u(t, x)$ with respect to t , u_{xx} is the second derivative of u with respect to x , u is a membrane potential in a nerve axon, the steady state $u = 0$ represents the resting state of the nerve.

Now if we map $u(x, t)$ into a CNN layer such that the state voltage of a CNN cell $v_{xkl}(t)$ at a grid point (k, l) is associated with $u(kh, t)$, $h = \Delta x$ and using the one-dimensional discretized Laplacian template A_1 , it is easy to design the CNN model of the proposed FitzHugh-Nagumo equation (10):

(1) CNN cell dynamics:

$$(11) \quad \frac{du_j}{dt} - I_j^s = u_j(u_j - \Theta)(1 - u_j) - b \int_0^t u_j(s) ds.$$

(2) CNN synaptic law:

$$(12) \quad I_j^s = \frac{1}{h^2}(u_{j-1} - 2u_j + u_{j+1}).$$

Let us assume for simplicity that the grid size of our CNN model is $h = 1$ and let us denote the nonlinearity $n(u_j) = u_j(u_j - \Theta)(1 - u_j)$. Substituting (12) into (11) we obtain:

$$(13) \quad \frac{du_j}{dt} - (u_{j-1} - 2u_j + u_{j+1}) = n(u_j) - b \int_0^t u_j(s) ds, 1 \leq j \leq N.$$

Equation (13) is actually integro-differential equation which is identified as the state equation of an autonomous CNN made of $N \times N$ cells [5,6].

General reaction-diffusion system is described by

$$(14) \quad \begin{aligned} \frac{du}{dt} &= D_1 \nabla^2 u(x) + F_1(u(x), v(x)), \\ \frac{dv}{dt} &= D_2 \nabla^2 v(x) + F_2(u(x), v(x)), \end{aligned}$$

where ∇^2 is two dimensional Laplace operator, D_1, D_2 are the diffusion coefficients, F_1, F_2 are the reaction models. Here we employ the Oregonators [1,5] for the reaction models:

$$(15) \quad \begin{aligned} F_1(u(x), v(x)) &= u(x)(1 - u(x)) - av(x) \frac{u(x) - b}{b + u(x)} \\ F_2(u(x), v(x)) &= u(x) - v(x). \end{aligned}$$

In this case the state variables $u(x)$ and $v(x)$ refer for the concentrations of two different chemical species at spatial position, a, b denote the reaction parameters. Depending on the reaction parameters, the Oregonator exhibits limit-cycle oscillations and excitatory behaviors. In the model, three types of reaction states are defined at one Oregonator, namely, inactive, active, and refractory states. When

the Oregonator is inactive, it is easily activated by an external stimulus, following which it changes to the refractory state. During the refractory state, the Oregonator cannot be activated even if an external stimulus is applied. Although D_1 is constant in general RD models, one may be more interested in a system where D_1 is locally modified by the potential gradient of $u(x)$.

In the next section we shall apply the local activity theory for the Oregonator RD-CNN model (14), (15).

3. Edge of chaos for Oregonator reaction-diffusion model

The theory of local activity [3,4] provides a definitive answer to the fundamental question: what are the values of the cell parameter for which the interconnected system may exhibit complexity? The answer is - the necessary condition for a nonconservative system to exhibit complexity is to have its cell locally active. The theory which will be presented below offers a constructive analytical method for uncovering local activity. In particular, for hysteresis CNN, one can determine the domain of the cell parameters in order for the cells to be locally active, and thus potentially capable of exhibiting complexity. This precisely defined parameter domain is called the edge of chaos. Recent laboratory observations suggesting that chaotic regimes may in fact represent the ground state of central nervous system point to the intriguing possibility of exploiting and controlling chaos for future scientific and engineering applications.

We propose the following constructive algorithm for studying the dynamics of Oregonator reaction-diffusion system (14), (15).

1. Map the Oregonator reaction-diffusion model (14), (15) into its discrete-space version by choosing the Laplace template of the following type $A_2 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{pmatrix}$. Then the reaction-diffusion CNN (RD-CNN) model of (14), (15) takes the form:

$$(16) \quad \begin{aligned} \frac{du_{ij}}{dt} &= D_1 A_2 * u_{ij} + u_{ij}(1 - u_{ij}) - av_{ij} \frac{u_{ij} - b}{b + u_{ij}} = G_1(u_{ij}, v_{ij}) \\ \frac{dv_{ij}}{dt} &= D_2 A_2 * v_{ij} + u_{ij} - v_{ij} = G_2(u_{ij}, v_{ij}) \end{aligned}$$

2. Find the equilibrium points E_k of (16) [7], which satisfy the system:

$$(17) \quad \begin{aligned} G_1(u_{ij}, v_{ij}) &= 0, \\ G_2(u_{ij}, v_{ij}) &= 0. \end{aligned}$$

In general, this system may have four real roots as functions of the cell parameters. We shall consider the equilibrium point $E_0 = (0, 0)$.

3. Calculate the cell coefficients $a_{11}(E_0)$, $a_{12}(E_0)$, $a_{21}(E_0)$, $a_{22}(E_0)$, of the Jacobian matrix at each equilibrium point.

4. Calculate the trace $Tr(E_0)$ and determinant $\Delta(E_0)$ of the Jacobian matrix at an equilibrium point E_0 .

Remark. It is very important to have circuit model for the physical implementation. Then we can apply results from the classical circuit theory in order to justify the cells local activity. If the cell acts like a source of small signal for at least one equilibrium point then we can say that it is locally active. In this case the cell can inject a net small-signal average power into the passive resistive grids [3,4].

We shall define stable and locally active region for the RD-CNN model (16).

Definition 3. We say that the cell is both stable and locally active region at the equilibrium point E_0 for RD-CNN model (16) if

$$a_{22} > 0 \text{ or } 4a_{11}a_{22} < (a_{12} + a_{21})^2 \text{ and}$$

$$Tr(E_k) < 0 \text{ and } \Delta(E_k) > 0.$$

This region in the parameter space is called $SLAR(E_0)$.

5. Determine the so called edge of chaos for our RD-CNN model (16). According to [3, 4] edge of chaos (EC) is a region in the parameter space of a dynamical system in which emergence of complex phenomena and information processing is possible.

Until now the definition of this phenomena is known only via empirical examples. Below we give more precise mathematical definition for EC.

Definition 4. RD-CNN model (16) operates in edge of chaos regime if and only if at least one equilibrium point which is both locally active and stable exists.

Following above algorithm we proved the main theorem in this paper:

Theorem 1. RD-CNN model (16) operates in edge of chaos if and only if the following conditions are satisfied: $0 < a < 1$, $\forall b$. This means that there is at least one equilibrium point which is both locally active and stable.

Proof. According to (17) we shall consider the equilibrium point $E_0 = (0, 0)$. The four cell coefficients in this equilibrium point are respectively: $a_{11}(E_0) = 1$, $a_{12}(E_0) = a$, $a_{21}(E_0) = 1$, $a_{22}(E_0) = -1$. Then, following Definition 3 we have

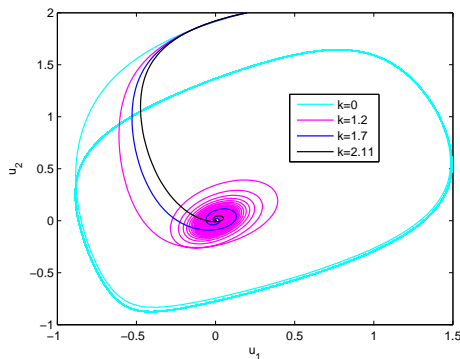


Figure 1: Edge of chaos domain in RD-CNN model (16)

that the condition $4a_{11}a_{22} < (a_{12} + a_{21})^2$ is satisfied in the equilibrium point $E_0 = (0, 0)$. The trace $Tr(E_0) = -1 < 0$ and the determinant $\Delta(E_0) = -1 - a > 0$ for $a < 1$. Therefore, the equilibrium point $E_0 = (0, 0)$ is both stable and locally active. Then according to Definition 4 we found the region of parameter set in which edge of chaos is determined. \square

On Figure 1 the edge of chaos region for RD-CNN model (16) is simulated for different parameter values.

4. Simulations and discussions

In the following simulations, a 2-D RD-CNN model with 100×100 Oregonators was introduced with a cyclic boundary condition [1]. The initial state of all the Oregonators was set to be inactive state. After stimulating the center node, the excitable waves propagated outwards, resulting in the generation of patterns of ocean surface waves. Figure 2 shows the time courses of the state u_{ij} depending on the direction of the wave propagation. According to the boundary conditions one can expect the waves to collide at the left-hand side and upward.

Then, instead of extraneous stimulus, the initial stimulation is changed by controlling the states of the Oregonators. In Fig. 3 several Oregonators next to the inactive Oregonators were initially set in a refractory state. When the inactive Oregonators were in an active or inactive state, the wave rotated inwards, which resulted in the generation of clockwise and counterclockwise spiral patterns. Depending on the direction of wave propagation, the velocity of the rightward and downward waves is faster than that of the leftward and upward waves. Over time, the initial position of the generated waves, is moved to the lower right.

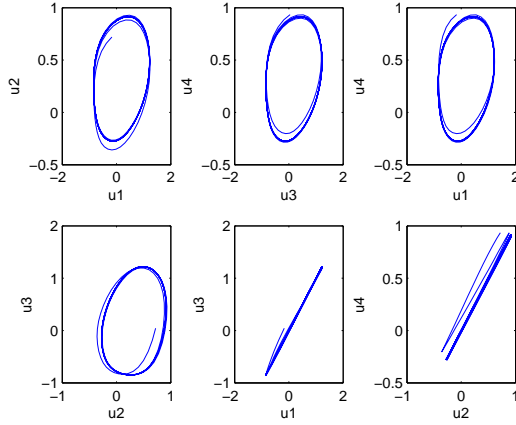


Figure 2: Simulations of four cells RD-CNN model (16) with cyclic boundary condition

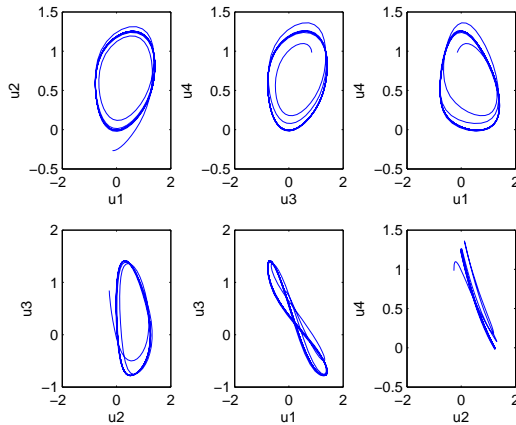


Figure 3: Simulations of four cells RD-CNN model (16) by controlling the states

Among the demonstrated behaviors, the nonuniform spatial-pattern generation can be applied in order to investigate and detect global motion of excitable waves. This results in detecting majority of wave directions at every spatial point. Therefore if one has proper RD media and a $2 - D$ array of RD-CNN without any reaction circuit, and the point dynamics of the RD media are given to this array, one may detect the global motions of the RD media. This application is

not limited in the analysis of RD systems, but the idea can be transferred to analyzing much more complex systems like brain networks, social networks, and so on.

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