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Differential Equation and Cellular Automata Model*

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Abstract

Cellular automata offered a promising modeling approach to simulate many complex systems. But researchers difficultly design suitable rules for models about real phenomena. And there is rich applied knowledge of differential equations in different fields. Researchers may model complex systems according to this knowledge from differential equations. This paper firstly survey correlative concepts about cellular automata and differential equations, and introduces general approach to design cellular automaton. According to tumor growth of Gompertz continuum differential equation, this article briefly discusses relations between cellular automata and differential equations, and builds a simple cellular automaton according to differential equations. At last this paper analyzes the results from mathematical viewpoint.

1 Introduction

In recent years, there are many researchers have interest on complex system science. Cellular automata (CA) are one of effective methods. CA consist of lots of discrete particles. From the theoretical viewpoint, Neumann and Ulam introduced CA in the late 1940's. John Horton Conway's "game of life" strongly attracted people's attention in the late 1960's. Wolfram did lots of work on non-linear dynamical theory of CA up to 1980's, and made a good base for physics models. A more systematic way in investigating the space of CA rules than Wolfram's phenomenological approach was opened by the parametric approach, at first gone by Langton[1]. CA are the discrete dynamical system in nature. It is composed by lots of simple components with local interaction each other. Its discrete character show that time, space and properties of the model just have only a finite number of states. CA can produce complex emergent behaviour by a lot of simple elements with local interactions according to simple rules. CA have been successfully used to model tumor growth, fluid flow, galaxy formation, biological pattern formation, civil development, avalanches, traffic jams, parallel computers, image processing, earthquakes and many more. In general, researchers regard CA as an alternative to differential equations (DE) in modelling physics. Due to many historical advantages and upon itself, until today, DE still has important status in modelling field. As we know, although Neumann had introduced the cellular automata theory many years ago, but it became important as a method for modelling and simulation of complex systems in recent years. The key reason is to the implementation of cellular automata on massively parallel computers. CA don't try to describe a complex system from a global point of view as it is described using DE, but modelling it starting from interaction of many individuals[2]. It brings an embarrassed problem for DE application. On the one hand, we construct continuity DE equations from the whole viewpoint; on the other hand, we have to spend much effort disable these 'advanced features' so that we can get our job done in spite of them[3]. Researchers require new modelling tools to make up this conflict, and CA may be suitable for modern computer further. How to take advantage of knowledge of DE and simple rules of CA is an important problem people take care in next step. Toffoli have discussed the relations between CA and DE[4]. And Omohundro studied opposite problem, i.e., how to model CA with DE [5].

In this paper, the first is to introduce necessary concepts about CA and DE. Then the second is to show the transition process from DE to CA. The third is to regard Gompertz DE describing tumor growth as an example to show the relations between two modelling tools, and design the CA model according to first-order DE. At last, we discuss statistic feature of CA from mathematical viewpoint.

2 General Approach

2. 1 Cellular Automata

CA is ideal mathematical model with discrete time and space. It may be described by five variables.

Definition 1: A standard CA is a quintuple set in *Eq.1*.

$$\text{Cellular Automaton}=\{\textit{Cells, Cell Space; Cell State, Neighborhoods, Rules}\} \quad (1)$$

where

(1) Cells: element of CA, shortening C;
(2) Cell Space: the set of all cells, i.e., state space of CA, and shortening: $S=\mathbf{Z}^d$;
(3) Cell Space: state a of cell at arbitrary time, and shortening local configuration: $d \in a^N$, then shortening global configuration: $c \in a^S$;
(4) Neighbors: neighbors of center cell, i.e., definition field, shortening: $N=\{n_1, n_2, \ldots n_k\}$;
(5) Rules: evolving rules of system, i.e., transition functions of cell states, shortening: $f: a^N \rightarrow a$.

The CA is a conceptual simple and effective solver for

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dynamic complex system. From common computer simulation viewpoint, a CA model provides an execution mechanism that evaluates the temporal dynamic behaviour of a dynamic complex system. Form a modeler's viewpoint, a cellular automaton model allows the formulation of a dynamic complex system application in simple rules. Based on standard CA, there are of course many corrective and extended computational models for different applied objectives. According to simple local transition functions, CA are intuitively regarded as a set of interacting elements are updated during a discrete time interval. In 1991, Weisbusch once defined a general CA into three discrete sets, such as *Fig. 1*.

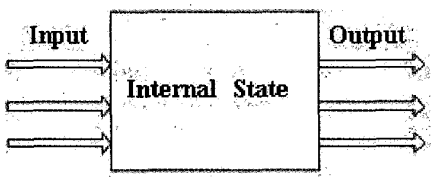

Figure 1: a general cellular automata

In total, there are three sets in a CA model, the set of inputs I, the set of internal states S and the set of outputs O. Meanwhile there are two mappings the state transition function $S(i,s)$ and the output function $O(i,s)$. In general, there are many inputs $i \in I$, internal states $s \in S$ and outputs $o \in O$. So mapping $S(i,s)$ and $O(i,s)$ are functions of the vectors i, s and o. CA are of course reduced further into two discrete sets, by considering the internal state and the output the same. Then the set of inputs I, outputs O and transition function $S(i,s)$ are composed into whole model $I \xrightarrow{S(i,s)} O$. A CA is the important tool for studying dynamical complex system. The most stunning feature of CA is the simplicity of the rules, which produce complicated, or self-organizing, behavior. To compare with those ordinary modeling approaches of DE, CA have many advantages in modeling field, such as discrete time, finite states, simple local rules and the inherent parallelism etc. Of course it is very difficult to produce quantitative results with CA without losing the simplicity and vividness of rules. Although the CA theory was introduced many years ago, due to the implementation of CA on parallel computers, in recent years it becomes significant as an approach for modeling and simulating of complex systems.

2. 2 The Transition Process

Most physics models, engineer models and biological models base on continuum variables of DE. If people want to take advantage of new CA approach, they must know the relations between CA and DE. There have been about 300 years since DE was applied in modelling. Users accumulate rich experiences in development process. Whereas, CA are the new-style approach suitable for modern computer tool. A DE may be approximated by a finite difference equation (FDE). This FDE in turn can be regarded as a cellular automaton. Then a cellular automaton is regarded as a system of extreme discrete DE. The process of continuous time into discrete interval corresponds to the transition process of DE into a finite difference equation. Here is a typical DE, such as *Eq.2*.

$$\frac{dx}{dt} = f(x, y) \tag{2}$$

The first phase is to transform DE into FDE, such as *Eq.3*.

$$x(t+1) = x(t) + f(x(t), y(t)) \tag{3}$$

The next phase is to replace all of the real variables x and y by discrete state variables of CA, then limit these variables into finite scope. So state variables are showed by finite small sets. At last, the operator $1+f$ of the FDE becomes the state transition function of CA with two inputs x and y. We may design evolving rules of CA according to the FDE and other knowledge. CA system evolves during a discrete time interval, and update the state variable x according to the state function of system, by means of the states of local neighbors and itself at present time. This transition process is depicted in *Fig.2*.

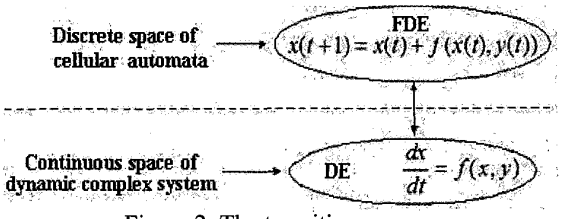

Figure 2: The transition process

In brief, the viewpoint of modelling physics system of CA is different from DE's; the property of variables the model depend on is different each other; Computational features of system is also different. In other words, a CA doesn't describe a complex system with complex equations, but model them with interaction of simple components according to simple rules. We may realize a complex system can be modelled by high-performance CA, and get good computing efficiency. They, CA and DE, are two kinds of modelling approaches in different space. In fact a CA is the DE in extreme discrete space. Wolfram had confirmed there are complex dynamical properties in discrete mathematical CA model, and absolutely implement relevant algorithms. Based on Wolfram's work, CA have been successfully used to model many variety complex systems, such as biology, chemistry, mathematics, physics field.

3 Using a Cellular Automaton to Simulate Tumor Growth According to Differential Gompertz Equation

3. 1 CA of Differential Gompertz Equation

Now we make a special example in tumor growth for showing the transition process in last sect. As we know, The Gompertz equation was developed by Gompertz for studies on human mortality at 1825. In 1934, Albert Casey was the first to use the Gompertz curve to fit tumor growth[7]. The Gompertz model is the best-known mathematical equation for modeling tumor growth most researchers prefer choose it. The differential Gompertz equation is given by *Eq.4*.

$$\begin{cases} \frac{dV}{dt} = V(\frac{A}{B})(1-(1-B)\exp(-Bt)) \\ V(t=0) = V_0 \end{cases} \quad (4)$$

where t is time; V is the tumor volume at time t; V_0 is the initial tumor volume; A and B are arbitrary constants parameters of model. The Gompertz model clarifies an evident fact that the volume V of the tumor is a function of time t. Whose solution is *Eq.5*.

$$V(t) = V_0 \exp\left[\left(\frac{A}{B}\right)(1-\exp(-Bt))\right] \quad (5)$$

whose derivation calculus is *Eq.6*.

$$\frac{dV(t)}{dt} = AV_0 \exp(-Bt)\exp\left(\frac{A}{B}(1-\exp(-Bt))\right) \quad (6)$$

The difference form of the Gompertz model can be derived from Eq.6 by dispersing the differential Gompertz model. Assuming T_0 is small enough, then the derivative of $V(t)$ with respect to t can be represented approximately as *Eq.7*.

$$\frac{dV(t)}{dt} \approx \frac{V(t+T_0)-V(t)}{T_0} \quad (7)$$

where t is discrete time, i.e., $t = kT_0$ ($k = 1,2,\ldots$), and T_0 is the discrete time interval. Accordingly, whose FDE is *Eq.8*.

$$V((k+1)T_0) = V(kT_0) + AV_0T_0 \exp(-BkT_0)\exp\left(\frac{A}{B}(1-\exp(-BkT_0))\right) \quad (8)$$

The discrete Gompertz model represented with *Eq.8* underlies the Gompertz CA, to be exactly, the stochastic evolutionary rules of the Gompertz CA. We may thereby get where $\Delta V_{CA}(t)$ is the ideal increment in the volume of the tumor simulated by the Gompertz CA at discrete time t in *Eq.9*.

$$\Delta V_{CA}(t) = \Delta V(t) = V(t+T_0) - V(t) = AV_0T_0 \exp(-BkT_0)\exp\left(\frac{A}{B}(1-\exp(-BkT_0))\right) \quad (9)$$

For one-dimensional CA growth model, $\Delta V_{max}(t)$ is the probable maximum increment in the volume of the tumor simulated by the Gompertz CA at discrete time t at each discrete interval. It is evident that there are just two Gompertz CA cells at every discrete time that probably evolve into tumorous Gompertz CA cells from normal Gompertz CA cells. Because of r_c (the probable maximum increment in the average radius of the tumor simulated by the Gompertz CA at discrete time t) is a constant, and then $\Delta V_{max}(t)$ is also a constant at any discrete time t in *Eq.10*.

$$\Delta V_{\max}(t) = 2\times V_c = \frac{8\pi}{3} r_c^3 = const \quad (10)$$

The evolution of the Gompertz CA cells has some uncertainty or randomness, which is characterized and quantified by the evolutionary probability. Given any $i \in \{-I_{\max},\cdots,-2,-1,0,1,2,\cdots,I_{\max}\}$, the evolutionary probability $p^{(i)}(t)$ of *Cell*(i) at discrete time t is defined in *Eq.11*.

$$p^i(t) = \begin{cases} 0 & s_{i-1}(t)=0 \quad and \quad s_{i+1}(t)=0 \\ 1 & s_{i-1}(t)=1 \quad and \quad s_{i+1}(t)=1 \\ \Delta V_{CA}(t)/\Delta V_{\max}(t) & otherwise \end{cases} \quad (11)$$

where $s_i(t)$ is the state of cell. The state of any CA cell is not reversible, i.e., it is not able to evolve into zero from one but into one from zero. Based on the discrete Gompertz model represented with *Eq.(8)*, the evolutionary rules of the Gompertz CA is defined in *Eq.12*.

$$s_i(t+T_0) = \begin{cases} s_i(t) & p^{(i)}(t) \le P_T \\ s_i(t)+1 & otherwise \end{cases} \quad (12)$$

where P_T the probable threshold belonging to [0,1] and generated with a uniform probability density function. In finite space, we just need simply code the initial conditions and evolving rules of CA. When the suitable time interval and the radius of cells in the CA model are chose, the dynamical properties of CA is in agreement with those features in DE.

3. 2 Analysis Statistics Feature of CA

In this sect, we will simply analyse the mathematical property of CA. In one-dimensional model case, there are just two Gompertz CA cells at every discrete time that probably evolve into tumorous Gompertz CA cells from normal Gompertz CA cells, and their state variables are described as $s_i(t)$ is random variable. The state of CA model is changing with evolutional rules. As we know, the relation is linear between the volume V and radius r of solid tumor. So the evolutionary probability $p^{(i)}(t)$ of *Cell*(i) at discrete time t can be defined in *Eq.13* again.

where ΔR_{CA} is the radius increment of CA model; and ΔR_{max} is the probable maximum radius increment. The volume V and radius r of solid tumor simulated by CA model is manifestly function of the volume increment $s_i(t)$. Thus, they are also random variables, and described as $\tilde{V}(t)$ and $\Delta\tilde{V}(t)$. According to the mechanism of tumor growth simulated by CA model, the random process of volume $\left\{ \tilde{V}(t) \mid t = kT_0, (k = 0,1,2,\cdots) \right\}$ is a Markov process without aftereffect, i.e. the state of random variable $\tilde{V}(t)$ at next time is to just relate with the sate at present time, and be foreign to other states at past time. This

process is described as *Eq.14*。

$$P\left(\tilde{V}(t+T_0)\,|\,\tilde{V}(t),\tilde{V}(t-T_0),\cdots,\tilde{V}(T_0),\tilde{V}(0)\right) = P\left(\tilde{V}(t+T_0)\,|\,\tilde{V}(t)\right) \quad (14)$$

where t is discrete time, i.e., $t = kT_0$ (k = 1, 2,...); T_0 is the discrete time interval; and $P\left(\tilde{V}(0)=V_0\right)=1$. Based on two random processes of the volume and the volume increment of CA model, we build FDE as *Eq.15*.

$$\tilde{V}(t+T_0)=\tilde{V}(t)+\Delta\tilde{V}(t) \quad (15)$$

The mathematical expectation of random process of volume $\left\{\tilde{V}(t)\,|\,t=kT_0,(k=0,1,2,\cdots)\right\}$ is important statistics property of CA model. $V_{CA}(t)$ is the ideal volume of tumor growth simulated by CA model at discrete time t. We suppose $\tilde{V}(t)=V_{CA}(t)$, and then there are three probable results of random variable $\Delta\tilde{V}(t)$, i.e., 0, $\Delta V_{\max}(t)/2$, $\Delta V_{\max}$. According to parallel evolving rules of CA model, $s_{i-1}(t)$ and $s_{i+1}(t)$ are independently random variables each other. Thus, we know as *Eq.16, Eq.17* and *Eq.18*, in view of Markov process *Eq.14*.

$$\begin{aligned}P\left(\Delta\tilde{V}(t)=0\right)&=P\left[\left(s_{i-1}(t)=0\right)\cap\left(s_{i+1}(t)=0\right)\right]\\&=P\left(s_{i-1}(t)=0\right)\cdot P\left(s_{i+1}(t)=0\right)\\&=\left(1-p^{s_{i-1}(t)}(t)\right)\cdot\left(1-p^{s_{i+1}(t)}(t)\right)\\&=\left(1-\frac{\Delta V_{CA}(t)}{\Delta V_{\max}(t)}\right)^2\end{aligned} \quad (16)$$

$$\begin{aligned}&P(\Delta\tilde{V}(t)=\Delta V_{\max}(t)/2)\\&=P\left\{\begin{array}{l}[(s_{i-1}(t)=1)\cap(s_{i+1}(t)=0)]\cup\\ \quad[(s_{i-1}(t)=1)\cap(s_{i+1}(t)=0)]\end{array}\right.\\&=p^{s_{i-1}(t)}(t)\cdot\left(1-p^{s_{i+1}(t)}(t)\right)+\left(1-p^{s_{i-1}(t)}(t)\right)\cdot p^{s_{i+1}(t)}(t)\\&=2\frac{\Delta V_{CA}(t)}{\Delta V_{\max}(t)}\left(1-\frac{\Delta V_{CA}(t)}{\Delta V_{\max}(t)}\right)^2\end{aligned} \quad (17)$$

$$\begin{aligned}P\left(\Delta\tilde{V}(t)=\Delta V_{\max}(t)\right)&=P\left[\left(s_{i-1}(t)=1\right)\cap\left(s_{i+1}(t)=1\right)\right]\\&=P\left(s_{i-1}(t)=1\right)\cdot P\left(s_{i+1}(t)=1\right)\\&=p^{s_{i-1}(t)}(t)\cdot p^{s_{i+1}(t)}(t)\\&=\left(\frac{\Delta V_{CA}(t)}{\Delta V_{\max}(t)}\right)^2\end{aligned} \quad (18)$$

Suppose the mathematical expectation $E\left(\tilde{V}(t)\right)=V_{CA}(t)$, well, now we prove it with the mathematical induction. When $k=1$, we may know as *Eq.19*, according to *Eq.16-Eq.18*.

$$\begin{aligned}E\left(\tilde{V}(T_0)\right)&=E\left(\tilde{V}(0)\right)+E\left(\Delta\tilde{V}(0)\right)\\&=V_0+\frac{\Delta V_{\max}(0)}{2}\times P\left(\Delta\tilde{V}(0)=\frac{\Delta V_{\max}(0)}{2}\right)+\\&\qquad\Delta V_{\max}(0)\times P\left(\Delta\tilde{V}(0)=\Delta V_{\max}(0)\right)\\&=V_0+\Delta V_{CA}(0)\\&=V_{CA}(T_0)\end{aligned} \quad (19)$$

When $k=1$, the supposition comes into existence. When $k\le K$, we suppose the supposition comes into existence at arbitrary discrete time $t=kT_0$. Then when $k=K+1$, we know as *Eq.20*.

$$\begin{aligned}E\left(\tilde{V}(t+T_0)\right)&=E\left(\tilde{V}(t)\right)+E\left(\Delta\tilde{V}(t)\right)\\&=V_{CA}(t)+\frac{\Delta V_{\max}(0)}{2}\times P\left(\Delta\tilde{V}(t)=\frac{\Delta V_{\max}(t)}{2}\right)+\\&\qquad\Delta V_{\max}(t)\times P\left(\Delta\tilde{V}(t)=\Delta V_{\max}(t)\right)\\&=V_{CA}(t)+\Delta V_{CA}(t)\\&=V_{CA}(t+T_0)\end{aligned} \quad (20)$$

The supposition comes into existence yet. So $E\left(\tilde{V}(t)\right)=V_{CA}(t)$ comes into existence at arbitrary discrete time $t=kT_0$. At last, CA model is agreement with the discrete tumor growth equation in the mathematical expectation $E\left(\tilde{V}(t)\right)$ sense. It means the difference form of differential Gompertz equation describing tumor growth process regards CA model as its mathematical expectation. In other words, CA model based on the finite difference Gompertz equation is agreement with the differential Gompertz equation.

4 Conclusion

The cellular automaton is the new-style, high-performance simulation tool, but designing rules always is difficult enough for real physics system. Even if in simple modelling case, there will be a great number of states in the cellular automata model. For example there is in total $2^{29}\approx10^{50}$states in Conway's "game of life". It is a very hard work to search suitable rules in this universal space. To build cellular automata model, researchers should take advantage of existent modelling approaches and relevant knowledge to look for good rules. Understanding the relation between CA and DE is helpful for application in different fields, and build a bridge between microscopic rules and macroscopic observation. As was shown in this article, a DE may be approximated by a FDE. This FDE in turn can be regarded as a cellular automaton, because of the introduction of finite difference and discrete variables. In some cases CA show high performance in modelling, in other cases people prefer the high precision of quantitative estimation resulting from DE. So we don't discuss which one, CA and DE, is better; just study the transition process from DE to CA, and show the process of designing the CA model for differential Gompertz equation simulating tumor growth. We hope researchers can bring into play well the modelling power of the CA approach in future in variety complex systems.

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