Computer Simulation of Shape Evolutions of Plant Cells Based on Physical and Chemical Interactions

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***Abstract*—Conventional computer modeling and visualization of plant tissues and cells are aimed at establishing corresponding static simulation models. In exploring the morphological evolution of cells in a microenvironment, interdisciplinary approaches need to be adopted to solve the underlying issues of dynamic modeling of cellular evolution. This study employs the reaction-diffusion equation to simulate the chemical signals driving cell growth. The Lattice Boltzmann Method (LBM) is used to obtain the expression for the incompressible fluid surrounding the cells, and the Immersed Boundary Method (IBM) is employed to simulate the cytoskeleton–flow field interaction. The visualized simulation of the interaction between the cell morphology and flow field is eventually realized using C++ and OpenGL 2.2. Experimental results suggest that the morphological evolution of plant cells can be realized by adjusting the fluid control parameters of the microenvironment, simultaneously proving the applicability of the proposed method as a computing mode for research in plant cell morphologies.**

Keywords—plant cells, Lattice Boltzmann Method, Immersed Boundary Method, cell morphology, computer simulation

I. INTRODUCTION

British biologist Thompson first published "On Growth and Form" in 1917, which is considered as the first critical moment for modeling the formation and development of organisms aided by mathematical knowledge [1]. In this work, Thompson expounded the shape, and scale of animals and plants as well as the surface tension of the membrane structure (such as cells) similar to soap, and demonstrated the geometrical shape of animal skulls on the Cartesian grid by means of the "Thompson conversion method". The conversion method is performed without considering the formation and differentiation of new organs, although it is related to initial and mature stages of organism development [2]. The restriction remained unsolved until the end of the 1960s. In 1968, Hungarian biologist Aristid Lindenmayer developed a set of formal languages to simulate the behaviours of plant cells. The language, also known as L-systems [3], is similar to Chomsky's production language, which is to establish a mathematical model of cell interaction at the cellular level using straight lines and branch structures to describe the morphogenesis of organisms. The computer model based on L-systems was not applied to the study on the development morphology of plant organs until the mid-70s. At that time, a computer model was developed for the relationship between plant development local organization and overall morphology and its information transfer [4].

The brief history of morphogenesis of organisms with geometric description was introduced above. Besides, there is another type of model that is established on the basis of the reaction-diffusion theory. To be specific, the model is adopted to represent the reaction-diffusion process of chemical substances from initial uniform and stable distribution state to the spontaneous formation from high concentration to low concentration. The theory was proposed in 1952 by the famous British computer scientist Alan Mathison Turing who attempted to explain the morphogenesis of natural organisms through establishing a series of reaction-diffusion differential equations [5]. Besides, Gernher and Mainhardt used short-distance activation and long-distance inhibition to recognize concentrations of the activator, and the inhibitor as well as the source density based on the "reaction-diffusion" theory. Specifically, when the source density is changed slowly, patterns are formed rapidly by concentrations of the activator and the inhibitor [6]. Moreover, Liao et al. obtained the equation exclusive for leopard markings using the reaction diffusion theory and experimentally demonstrated that markings of leopard in the development stage can be displayed through changing the parameters in the equation and computer calculation [7].

Cell morphology and quantity directly contributes to the composition of plant leaves, while the mechanical force that is primarily produced by the reaction-convection-diffusion of substances inside and outside the cell is a major cause for its morphogenesis [8][9]. On this basis, the evolution of cell morphology is modeled to provide a mathematical explanation for describing cell growth via computer from the physical-chemical perspective.

II. METHODS

The cell evolution process is decomposed into a structure consisting of chemical level, physical layer and geometric representation due to its complexity, as shown in Fig. 1.

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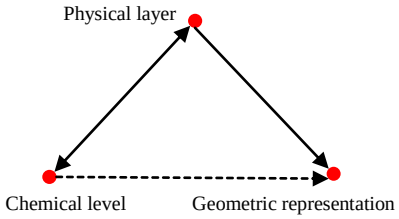


Fig. 1. Physical-chemical interactions in cell morphological evolution modeling

A. Key technologies at the chemical level. The reaction-diffusion differential equation is simulated at the chemical level using biological signals of cell growth in the chemical layer. Its vector form is shown in Eq. 1. Moreover, the solution is conducted in a Cartesian grid or Euler grid resorting to the D2Q5 model of the lattice Boltzmann method [10].

$$\frac{\partial \rho_s}{\partial T} - D_s \nabla^2 \rho_s = R_s \qquad (1)$$
$$1 \le s \le M$$

where, T is the time; ∇^2 is the Laplace operator related to the specific space X ; M is the species number of substance; $\rho_s(X,T)$ is the mass density of the substance s at the time T and the location X ; D_s is the diffusion coefficient; and R_s is a reaction term that is dependent of the density of the reaction of ρ_s and s with other substances.

B. Key technologies at the physical level. In this paper, the movements of flow field of the cell wall and its boundary were simulated with the help of the immersed boundary in accordance with the basic idea of converting the boundary into a body force in the Navier-Stokes viscous Newtonian fluid equation [11]. Assuming that the fluid in the physical layer is incompressible and viscous with consistent viscosity inside and outside the cell, its two-dimensional Navier–Stokes equation is presented in Eq. 2.

$$\rho\left(\frac{\partial u}{\partial t} + u \cdot \nabla u\right) = -\nabla p + \mu \Delta u + F \qquad (2)$$
$$\nabla \cdot u = 0$$

where, ρ is the constant fluid density; μ is the hydrodynamic coefficient of viscosity; u is the fluid velocity; p is the fluid pressure; F incorporates all the body force transmitted from the cell wall boundary to u . And F is defined in Eq. 3.

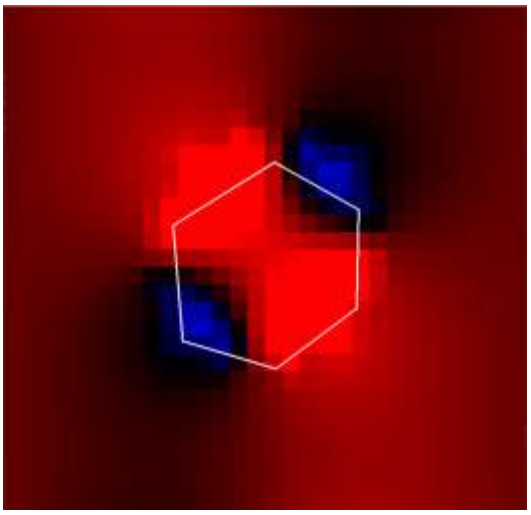
$$F(x,t) = \int f(q,s,t)\delta(x - X(q,s,t))\delta(y - X(q,s,t))ds \qquad (3)$$

where, $f(q,s,t)$ is the unit force resulted from the immersed boundary; $X(q,s,t)$ is the boundary coordinates at t time; and δ is the Delta Dirac function. The solving process is performed in the same way as the chemical level, that is, the force F is mapped to the Cartesian grid using the D2Q9 model of the lattice Boltzmann method.

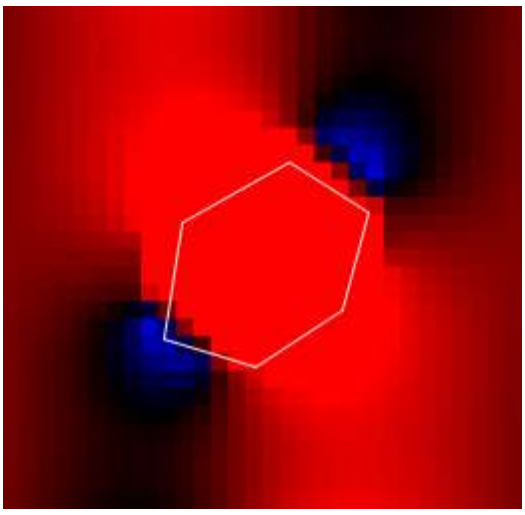
C. Key technologies at geometric representation. The vertex coordinate of the original shape of the cell is calculated using the immersed boundary method. To begin with, the body force is calculated based on mechanical equations together with the vertex position at the boundary of the cell shape. Then, forces at the node of surrounding fluids are deduced from the body force. After that, the flow control equation is solved as per the force at the grid node of the fluid field. Finally, the new coordinates for the vertex of the cell shape can be obtained with the adoption of new velocity field distribution.

III. Experiment and Discussion

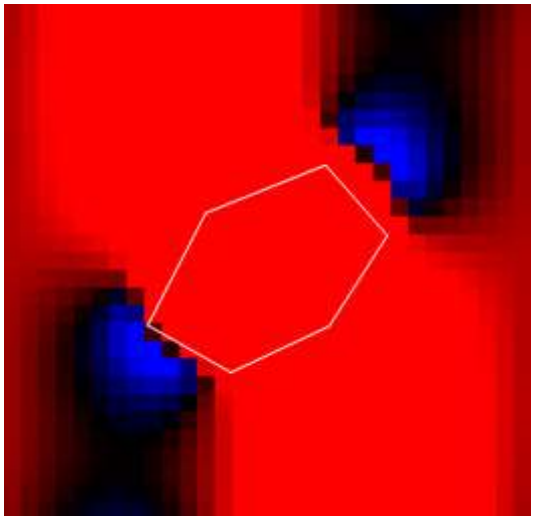
I5-8300H 2.30GHz CPU, and 16.0G memory were configured to the computer hardware in the experimental environment together with a 64-bit Windows 10 operating system, C++ programming language and OpenGL 2.2 graphics library. Meanwhile, the geometric boundary of a plant cell was fitted using a hexagon, and the flow field falls into a grid of 30×30 nodes. Concerning initialization parameters, relaxation time was set to 1; the force density resulted from gravity is 0; the velocity at the bottom wall of the flow field was -0.02; the velocity at the top wall was 0.02; the grid fluid viscosity μ was 0.1667, and the fluid Reynolds number Re was 0. Note that all units were dimensionless. When t =200, t =400, t =800, and t =1200 iterations, the cell visualization shapes are presented respectively in Fig. 2.



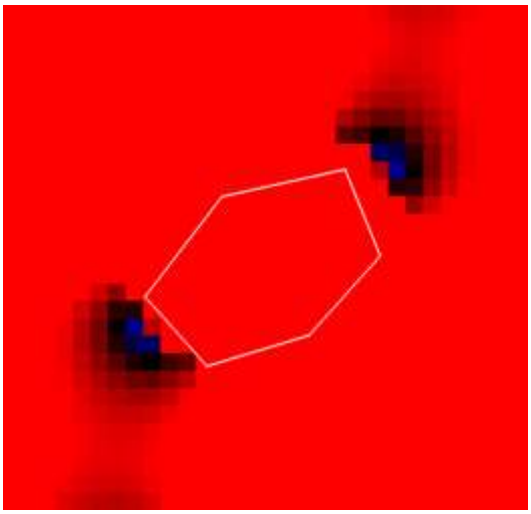
t=200



t=400



t=800



t=1200

Fig. 2. Visualization of plant cell model when t=200,400,800,1200 iterations.

Evidently, the fluid velocity is changed with the changed density of surrounding fluid, leading to variations in spots on the plant cell. The experimental results simulate the occurrence of morphological changes of cells under the effects of intracellular and extracellular spaces, achieving the diffusion and fluid effect of plant cell as well as the dynamic process of geometric representation.

IV. CONCLUSION

A physical-chemical modeling method is proposed to analyze and simulate the evolution of cell morphology, which can prevent from modeling and analysis of complex and temporarily unclear gene regulatory networks. In this study, one method is proposed to simulate the evolution of the two-dimensional visualization geometric model of plant cells in the flow field. What's more, a layered calculation approach is adopted in the proposed method, which can easily extend the problems that plant cells are not merely a three-dimensional structure, and the interaction between cells is not considered due to the effect of cell wall between cells.

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