A SYSTEM FOR SIMULATION OF 2D PLANT TISSUE GROWTH AND DEVELOPMENT

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SUMMARY

Motivation: At the tissue level growth and development are determined by cellular biomechanics, molecule transportation, and cellular responses to their microenvironments. Biologically motivated models of such processes, when incorporated into models of tissue growth and development, would help to study the roles of these processes in tissue growth and morphogenesis.

Results: A program system for simulation of "planar" plant tissue growth and development was developed. The system includes graphical user interface to prepare an initial configuration of system to be modeled and to perform simulations.

INTRODUCTION

Morphogenesis on the scales from cells - tissues - organs and up to the whole organism depends on differential cell growth and division. It is shown that deformation tensions that arise in different parts of growing biological tissue have dramatic effect on the all biological processes up to differential gene expression (Nelson et al., 2005). The gene expression controls the cell functions. Thus biomechanics and biological functions form a regulatory loop. While development processes including morphogenesis in animals involve cell movement, it dose not occurs in plants, so the plant tissue development is, in a sense, easier to model and simulate. The growth of plant cells and tissues is shown to be dependent on water potential in the cells. The growing plant cells are enveloped with primary cell wall, which can yield under intracellular pressure (Cosgrove, 1986).

We used models of the main biophysical processes in cells and tissue, which are listed above, to construct a model of plant tissue growth and a program system for its simulation.

METHODS AND ALGORITHMS

Biophysical considerations. (Nobel, 1973) Water flow between compartments with semipermeable boundaries is proportional to the difference between water potentials in the compartments:

$$\frac{dv_k}{dt} = \sum_{i(k)} (\psi_{i(k)} - \psi_k) \cdot L_{k,i(k)}, \quad (1)$$

where $L_{k,i(k)}$ is hydrodynamical conductance; and $i(k)$ are numbers of the cells in the neighborhood of the i-th cell.

Water potential is dependent on osmotic (π_k) and hydrostatic (turgor) (P_k) pressures:

$$\psi_k = P_k - \pi_k \quad (2)$$

In turn, osmotic pressure is dependent on content of osmotically active particles s_k in a compartment, the pressure for diluted solutions is:

$$\pi_k = \frac{s_k \cdot R \cdot T}{V_k}, \quad (3)$$

where V_k, R, T are the compartment volume, the absolute gas constant, and the Kelvin temperature respectively.

Applied pressure and volume for condensed matter obey to the state equation (Prigogine, Defay, 1966):

$$\upsilon(T, p) = \upsilon(T, 0) \cdot (1 - \kappa \cdot p) \quad (4)$$

where κ is thermodynamical compressibility, the typical value for liquids is $\sim 10^{-4} Bar^{-1}$; $\upsilon(T,0)$, $\upsilon(T, p)$ are molar volumes for reference (*0*) and an excess (p) pressures respectively.

The equation (4) is used to calculate intracellular hydrostatic pressures resulting from water flows (1). The pressures enforce deformation of the tissue, which consists of the cells.

There are cell wall deformations at the base of the deformation of the tissue. In a certain range of intracellular pressure, the cell wall deformation is elastic and above a threshold pressure this deformation is plastic –the cell wall behaves like viscous liquid. Elastic deformation obeys the Hooke's law: $T = \frac{E \cdot S \cdot \Delta l}{l}$. Viscous behavior is described as $\frac{dl}{dt} = \eta \cdot F$; appearing viscosity η reflects cellular capacity to remodel its walls, and F is the applied force.

The cell deformations arise as result of cell wall vertex movements caused by applied forces, as illustrated in Fig. 1 in the elastic case.

Features of calculation. The processes that are described in terms of different nature are involved in the model. For example, a process changes the system's topology (mainly, the cell divisions). Other processes are responsible for evolution of distributed system parameters such as the concentration of chemical substances (biomass growth, differential gene expression, and transport processes). It is convenient to use systems of ordinary differential equations to describe one kind of processes. The other processes are described as operations with algebraic structures like graphs. Operator formalism is used to unify these different approaches.

Each cell is represented as a polyhedron with straight elastic walls. Walls of neighbor cells are tightly bound to each other. Each wall separating two neighbor cells consists of two straight elastic rods (one for each cell) (Fig. 2).

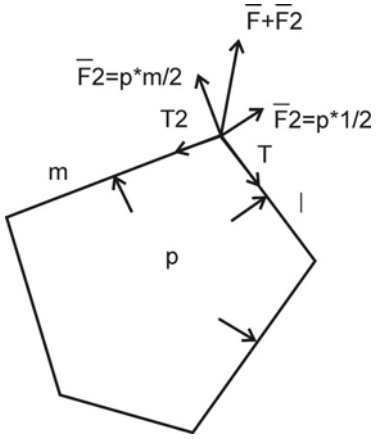

Figure 1. Vector diagram for forces on a cell wall vertex.

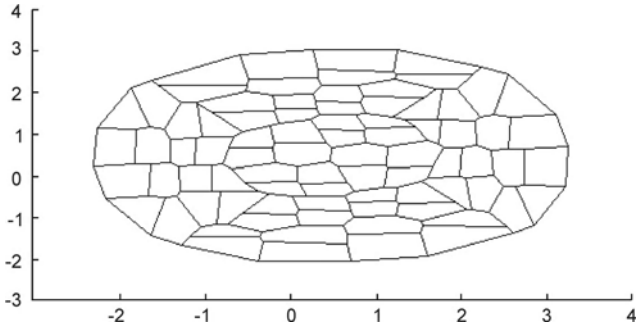

Figure 2. Spatial structure of a toy tissue.

The concentration of chemical substances can be different in different cells but it is considered to be uniform within a single cell. Some chemical substances can freely penetrate through the cell walls. The transport of the other substances is restricted.

Data structure of the model consists of the following groups of parameters: (a) global model parameters; (b) individual cell parameters such as topology, cell wall properties, and chemical cell contents; (c) vertex properties.

Let us demonstrate an example of an operator's inner structure. This operator describes the processes of mechanical deformation and turgor dynamics.

$$\vec{x}_i = \sum_{\substack{rod\ \vec{l}\\ incident\\ to\ vertex\ i}} k_{elastic} \cdot (\left|\vec{l}\right| - \left|l_n\right|) \cdot \frac{\vec{l}}{\left|\vec{l}\right|} \cdot \mathrm{sgn}(\vec{l}) + \sum_{\substack{rod\ \vec{l}\ from\ cell\\ incident\\ to\ vertex\ i}} \frac{1}{2} \cdot \frac{1}{k} (1 - \frac{1}{vp0} \cdot \frac{V_{cell}}{\mu_{cell}}) \cdot \left|\vec{l}\right| \cdot h \cdot \vec{n} \qquad (5a)$$

$$\dot{\mu}_k = \sum_{\substack{nigbor\ i\\ of\ cell\ k}} \left[\frac{h \cdot L_w}{k \cdot vp0} \cdot l(i,k) \cdot [\frac{V_k}{\mu_k} - \frac{V_i}{\mu_i}] \right] + \sum_{\substack{nigbor\ i\\ of\ cell\ k}} \left[h \cdot L_w \cdot RT \cdot l(i,k) \cdot [\frac{\mu S_k}{V_k} - \frac{\mu S_i}{V_i}] \right] \qquad (5b)$$

Here $\vec{x}_i$ are the coordinates of the vertex *i*, μ_k is molar water content in cell k, V_k is the volume of the cell *k* and the other variables are model parameters.

Another group of operators implements external interaction with the model. These are so-called dialog operators. They are implemented as User Interface.

IMPLEMENTATION AND RESULTS

The graphical user interface is an organizing component. It is designed to provide convenient interaction with the program. Its purpose is to join the stages of creation and development of cellular ensemble, and also to build and execute various scripts of cellular ensemble dynamics.

Interface components implements the following functions:

1. Creation of cellular ensemble geometry (Fig. 3), i.e. assignment of the initial parameters of ensemble formation in dialog with the user. The following parameters are defined: the number of the cells in ensemble, the shape of the ensemble, and also the cell geometry in the selected ensemble, that depends on topology of intercellular connections, definition of cell types, boundary cells, etc.
2. Marking of cellular ensemble, i.e. definition the fields of non-geometrical cell parameters and assignment values for them. The next parameters are definable: pressure inside a cell, levels of morphogens, osmotically active molecules, etc. These parameters determine model of intracellular dynamics.
3. The important function of interface component – Editing of the cellular ensemble (Fig. 5) during simulation. This function allows the user to change the parameters of the cells: intracellular pressure, levels of morphogens and other molecules concentrations, lengths of relaxed cell walls, vectors of growth and division.
4. The next module implements the interface with the process of simulation. (Fig. 4). It allows the user to execute scripts, specifying cellular ensemble dynamics using of various operators, and to track the results after each simulation step.
5. And the last function is the graphical representation of results of the current simulation: visualization of cellular ensemble parameters in dynamics, and static images of parameter fields in cellular ensemble. Useful options are supplied in the block, for example, representation of a chosen cell parameter in pseudo-colors (intracellular amounts of molecule of interest, cell wall tensions, thickness, permeability, etc.).

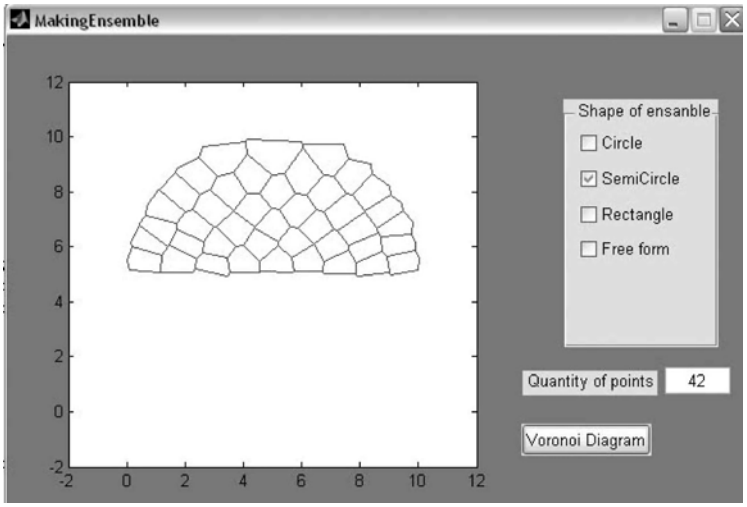

Figure 3. Initial geometry specification.

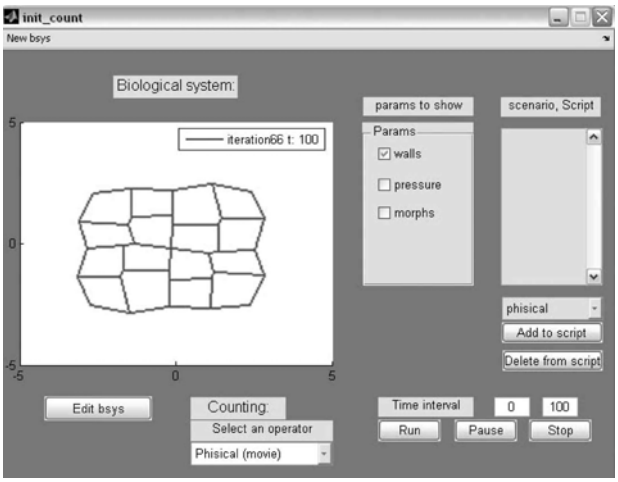

Figure 4. Model calculation

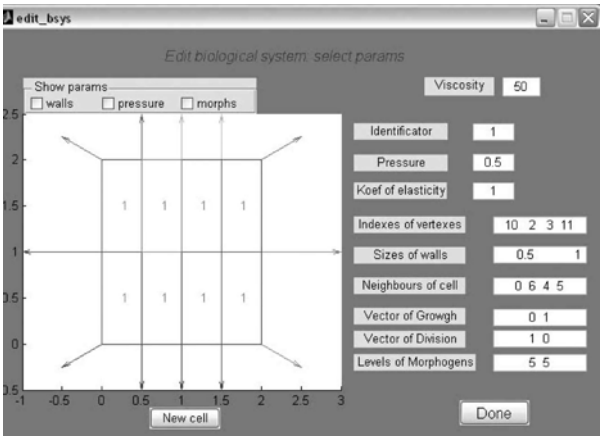

Figure 5. Modification of a cellular ensemble

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