Journal of Computational Science 9 (2015) 107–111

Contents lists available at ScienceDirect

Journal of Computational Science

journal homepage: www.elsevier.com/locate/jocs

Simulating leaf growth dynamics through Metropolis-Monte Carlo based energy minimization

Dirk De Vos[a,*], Emil De Borger[a], Jan Broeckhove[b], Gerrit T.S. Beemster[a]

[a] Department of Biology, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen, Belgium
[b] Department of Mathematics and Computer Science, University of Antwerp, Middelheimlaan 1, 2020 Antwerpen, Belgium

ARTICLE INFO

Article history:
Available online 17 April 2015

Keywords:
Computational biology
Leaf development
Growth simulation
Metropolis
Hamiltonian

ABSTRACT

Throughout their life span, plants maintain the ability to generate new organs, such as leaves. This is normally done in an orderly way by activating limited groups of dormant cells to divide and grow. It is currently not understood how that process is precisely regulated. We have used the VirtualLeaf framework for plant organ growth modeling to simulate the typical developmental stages of leaves of the model plant *Arabidopsis thaliana*. For that purpose the Hamiltonian central to the Monte-Carlo based mechanical equilibration of VirtualLeaf was modified. A basic two-dimensional model was defined starting from a rectangular grid with a dynamic phytohormone gradient that spatially instructs the cells in the growing leaf. Our results demonstrate that such a mechanism can indeed reproduce various spatio-temporal characteristics of leaf development and provides clues for further model development.

1. Introduction

Generally, the ability of plants to generate new organs, such as leaves persists during their life time by virtue of so called meristems. These structures typically are maintained by a group of slowly growing and dividing cells that can become activated to start faster proliferation and expansion [1,2]. Dicotyledons (or dicots) are a vast group of plant species with a common embryonic layout with the weed *Arabidopsis thaliana* arguably being the most important experimental model plant. In that capacity it is important to understand its growth and development. Typically, various stages or phases with a distinct profile of cell division and expansion can be distinguished in the development of its leaves. Although many molecules have been implicated in the regulation of leaf growth, there is still no definitive understanding of the mechanism governing the succession of those stages.

During the last decade or so computational modeling has become an increasingly important tool to understand complex processes in biology and in particular in plant physiology [3–5]. Different modeling platforms have been developed to facilitate construction and implementation of spatio-temporal models of plant development [6–8]. In a recent study Kuchen et al. proposed hypothetical models to explain differences in relative growth rate (strain rate) across the leaf blade of early growth stages of the *Arabidopsis* leaf (primordium) [9]. Here we make use of a vertex-based tissue modeling platform to develop an elementary model that can reproduce the major stages during *Arabidopsis* leaf development and at the same time can approximate quantitative growth characteristics from experimental data which are colloquially termed 'kinematics' [10,11].

2. Computational method

The VirtualLeaf C++ framework for modeling plant organ growth [8] was used as a starting point. It uses a vertex-based description of plant tissue with cells represented by polygons consisting of nodes or vertices connected by edges. The edges represent the cell wall segments and cell membranes that separate neighboring cells. All cells are interconnected in the cellular grid or mesh and neighboring cells remain connected. The inability for cells to slide relative to each other corresponds to the so called symplastic nature of living plant tissues.

Importantly, this mesh or cellular grid forms the cradle of a variety of biochemical processes which are specified in model specific classes. There the dynamics of chemical processes within the cells, within the walls and the transport processes between neighboring cells and between cells at the boundary and the external environment are described. These processes determine the evolution of the various biochemical components in the form of ordinary differential equations. Like in real tissue individual cells are also able to

* Corresponding author.
E-mail address: dirk.devos@uantwerpen.be (D. De Vos).

http://dx.doi.org/10.1016/j.jocs.2015.04.026
1877-7503/

increase in size (grow) and undergo division. The rules specifying growth and division are also described in model specific classes.

A second crucial part of the framework governs the cell mechanics. In accordance with normal plant tissue cells of the mesh are characterized by an internal pressure or turgor pressure that is counterbalanced by the tension of the surrounding walls. To find the equilibrated state for all cells in the tissue we apply a Metropolis algorithm [12]. We look for a mesh geometry that minimizes an objective function or a generalized energy function or Hamiltonian H that is defined as follows:

$$H = \lambda_A \sum_i \left(\frac{a(i) - A_T(i)}{a(i)} \right)^2 + \lambda_M \sum_j (l(j) - L_T(j))^2,$$

where indices i and j sum over all cells and polygon edges, respectively. The parameter λ_A sets the cells' resistance to compression or expansion, and parameter λ_M is a spring constant. A_T is the cell's target area, and L_T the wall element target length. a and l are the actual cell area and actual wall element length. The first term represents a turgor pressure potential of the cells whereas the second term an elastic (spring) potential energy. The first term is a modification of the original version [8] which scales the turgor pressure potential according to the cell areas, resulting in similar relative contributions to the Hamiltonian of cells with different areas. To find the equilibrium mesh geometry in the Metropolis approach all nodes are considered for displacement, one at a time in a random order. The random displacement vector is determined by two random numbers for horizontal and vertical displacement, respectively. If the displacement results in a decrease of energy H, then the displacement is accepted. To avoid getting stuck in a local energy minimum the displacement is also accepted with a probability given by the Boltzmann function:

$$P(\Delta H) = e^{-\left(\frac{\Delta H}{T}\right)},$$

with T a parameter setting the amount of noise.

The Metropolis algorithm is applied iteratively until the overall energy decrease for a sweep over all nodes remains below a predefined value. After the mechanical equilibration (example in Fig. 1) the simulation algorithm continues by numerical integration of all differential equations representing the biochemical processes, but based on the updated variables (cellular areas for instance have changed due to the Monte Carlo runs). Moreover, the rules for cell division and cell growth are also evaluated. This potentially leads to cell partitioning and an increase in the cells' target area. The function that specifies the (relative) increase in target area is crucial since it forces the cells to expand during the next Monte Carlo runs. As the cell walls are extended too by that process they eventually exceed a preset yield threshold. Consequently new nodes are introduced into that wall which represents the (real) process of irreversible wall yielding and allows further growth of the tissue in the next cycles.

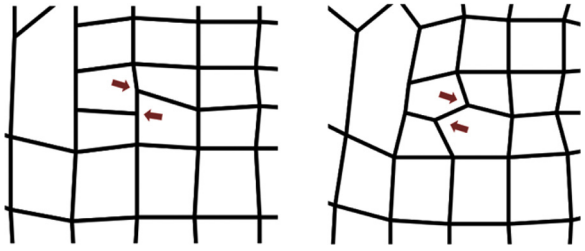

Fig. 1. Example of virtual plant tissue before and after mechanical equilibration.

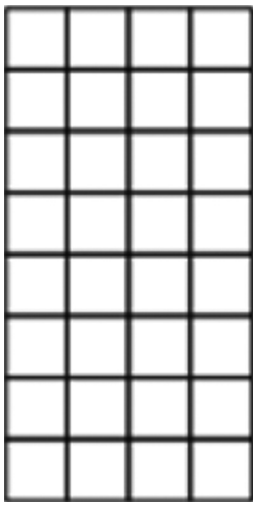

Fig. 2. Starting cell mesh.

3. Model description

The starting grid consisted of 32 square cells (Fig. 2), the top 16 representing the leaf blade and the bottom 16 representing the petiole. The latter have a fixed position assuming the blade is the major expanding part. To decrease the duration of the computations a limited number of starting cells were used with each cell equivalent to an ensemble of 64 cells. The start of the simulation was set to correspond to day 4 after sowing of the real *Arabidopsis* seedling and time steps of 4 h were taken until growth ceases across the leaf blade after roughly 20 days.

We have assumed that one biochemical compound (the morphogen) controls the developmental behavior of the cells. The morphogen is produced in the petiole cells at a constant rate for 5 days and is continuously degraded (or converted) proportionally to its concentration. The 'morphogen' is passively transported (diffused) throughout the tissue. The diffusion takes place on a cell-to-cell basis according to the following equation:

$$\frac{dM_i}{dt} = \sum_j \left[l_{ij} D \frac{\Delta c_{ji}}{\Delta x} \right],$$

which expresses the change of the number of molecules of the morphogen M in cell i over time as the sum of the diffusive fluxes from all neighboring cells j multiplied by the respective wall segment lengths l_{ij} (=lengths of the edges of the cell polygon). For the diffusion processes a discrete equation for Fick's law was used that expresses the diffusive flux as proportional to the diffusion coefficient D and to the concentration difference of the substance between cell j and cell i (Δc_{ji}), and inversely proportional to the thickness of the wall segment (Δx). The complete equation for cell i, then becomes:

$$\frac{dM_i}{dt} = \sum_j \left[l_{ij} D \frac{\Delta c_{ji}}{\Delta x} \right] + P - k_d M_i,$$

with $P = 0$ for cells of the blade. The cellular concentration of M determines the behavior of the individual cells. If a cell exceeds a specific threshold value and at the same time has reached a minimum size (area) the cell is instructed to divide. A different (lower) threshold value needs to be exceeded to drive a certain relative increase in the target area of that cell. These values are listed in Table 1.