Available online at www.sciencedirect.com

ScienceDirect

Procedia Computer Science 108C (2017) 139–148

Procedia Computer Science

International Conference on Computational Science, ICCS 2017, 12-14 June 2017, Zurich, Switzerland

Simulation of regulatory strategies in a morphogen based model of *Arabidopsis* leaf growth.

Elise Kuylen[1], Gerrit T.S. Beemster[2], Jan Broeckhove[3], and Dirk De Vos[4]

[1] University of Antwerp, Antwerpen, Belgium
elise.kuylen@student.uantwerpen.be
[2] University of Antwerp, Antwerpen, Belgium
gerrit.beemster@uantwerpen.be
[3] University of Antwerp, Antwerpen, Belgium
jan.broeckhove@uantwerpen.be
[4] University of Antwerp, Antwerpen, Belgium
dirk.devos@uantwerpen.be

Abstract

Simulation has become an important tool for studying plant physiology. An important aspect of this is discovering the processes that influence leaf growth at a cellular level. To this end, we have extended an existing, morphogen-based model for the growth of *Arabidopsis* leaves. We have fitted parameters to match important leaf growth properties reported in experimental data. A sensitivity analysis was performed, which allowed us to estimate the effect of these different parameters on leaf growth, and identify viable strategies for increasing leaf size.

Peer-review under responsibility of the scientific committee of the International Conference on Computational Science

Keywords: modelling and simulation, computational biology, leaf development

1 Introduction

Mathematical modelling and simulation is becoming increasingly important in the bio-sciences, particularly in the field of plant physiology. An important factor in this evolution from a reductionist towards a systemic approach, is the rapidly increasing knowledge on the molecular processes that determine the form and function of plants. Large-scale ('omics') studies at the level of DNA, RNA and proteins, as well as more focused studies, have deciphered more and more regulatory networks and pathways that govern cellular behaviour.

Since all cells in a plant are both biochemically and mechanically connected in a so-called symplastic framework, it is important for modelling studies to include spatial dimensions. To describe such a cellular grid - the plant tissue - in which cells are fixed with respect to their neighbours, several plant modelling platforms have been developed. Some of these are primarily aimed at the simulation of plant architecture and the interaction of plants with their environment [18, 8, 17], whereas others focus on the cellular level and the tissue level [6, 16]. The

1877-0509
Peer-review under responsibility of the scientific committee of the International Conference on Computational Science
10.1016/j.procs.2017.05.238

latter are vertex-based simulators that represent plant tissue as polygons of vertices that are connected by edges. These edges represent cell wall segments and have mechanical attributes. This makes these models highly suitable for simulating tissue and organ growth.

Functioning as its central power-station, leaves are the basis for growth of the plant. Improving our understanding of leaf growth and development can potentially lead to crops with higher productivity and resistance to climate change [11]. While many experimental approaches exist for studying leaf growth regulation from a molecular perspective, we should be able to quantify leaf growth in a precise way. Various methods exist for this purpose, depending on the plant species being studied. Quantifying the growth of the experimentally widely studied plant *Arabidopsis thaliana* typically involves measuring the evolution of the leaf area, estimating the total cell number and calculating a number of derived quantities. This has led to the distinction of different phases during leaf development. After the start the leaf (primordium) primarily grows by uniform cell division. A division front and afterwards an expansion-only front gradually develop. Over time, both fronts move to the leaf base. Eventually, the growth zones disappear from the leaf, and after cell maturation leaf growth is finished [7].

Mathematical models have been proposed for several aspects of leaf development such as leaf initiation [3, 19], shape [14], serration [2], and venation [20]. Previously, we proposed a computational model which reproduces the main stages of leaf growth based on a single mobile signal or morphogen that is produced at the base [5]. In this paper, we present a leaf growth model, which we improved using experimental data from Kheibarshekan Asl et al. [13]. These data precisely quantify the evolution of cell numbers and sizes over time. Through a sensitivity analysis the influence of perturbation of model parameters and their associated processes on leaf area, total cell number and average cell area is investigated.

2 Methods

2.1 Simulator framework

We have used a vertex-based simulator that has been developed in C++11, building on the VirtualLeaf framework [16]. The cells are modelled as polygons of nodes connected by edges, which represent the cell walls and membranes separating the cells in the tissue. Both cells and walls have attributes such as chemical concentrations or mechanical properties. Dedicated classes are used to implement the rules and equations that govern the dynamics of those attributes.

The simulator moves forward in discrete timesteps, the length of which can be specified through an input file. This input file also contains the initial conditions of the cellular mesh as well as all model parameters. During each timestep, two important processes are executed. First, biochemical processes within and between cells are simulated. This includes intracellular reactions, transport processes between cells, evaluation of rules for cell division and so forth, which are all described in model-specific classes. Subsequently, the mechanical movements of the tissue are simulated with displacements of all nodes in a Metropolis-Monte Carlo based energy minimization algorithm.

Leaf cells experience an internal (turgor) pressure that forces them to expand against the elastic forces from neighbouring walls. To find an equilibrium, we use a Metropolis algorithm (see [16] for details) to minimize an energy function (Hamiltonian) of the cell mesh. This Hamiltonian function can be expressed as follows:

$$H = \lambda_A \sum_i \left(\frac{a(i) - A_\tau(i)}{a(i)} \right)^2 + \lambda_M \sum_j \left(l(j) - L_\tau(j) \right)^2$$