

DyCeModel: a tool for 1D simulation for plant hormones control of tissue patterning using shoot and root apical meristems of *Arabidopsis thaliana* as examples

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Motivation and Aim: The question of the mechanisms of growth and development is very challenging. To do this, it is necessary to analyze changes in the regulators distribution throughout the tissue in time and space and take into account their influence on cellular dynamics within the tissue. The main regulators of cellular dynamics in tissues are plant hormones, which form gradients and maxima to control molecular processes depending on concentration. Previously mathematical modeling was successfully used to study the effect of the plant hormones concentration distribution on the plant stem cell niches functioning in 1D and 2D models, in which cell division, growth and differentiation were under the control of signaling molecules [1–5]. Nevertheless, these models remain within a specific meristem and are not suited to other plant stem cell niches. A common description of the main complex of processes associated with the redistribution of hormone concentrations and cell responses to them can serve as the basis for studying the general and specific characteristics of meristems in various plants. Therefore, one of the actual tasks is to create software that builds computer models of various plant organs using uniformly described processes and provides automatic adjustment of parameters. We have created the DyCeModel pipeline for one-dimensional tissue modeling with a dynamic cellular ensemble, where changes in the concentration of hormones (or other active substances) in cells are described by ordinary differential equations (ODEs).

Methods and Algorithms: The DyCeModel pipeline allows you to create a dynamic one-dimensional structure of cells, integrate it into a mathematical model in the form of an ODE, and conduct a computational experiment. It contains five script files (.m files) that run in the MATLAB software environment. The substance_eq.m file contains an ODE system for describing the synthesis, degradation, passive and active transport of substances of interest. By default, DyCeModel provides examples of functions describing these processes for two substances in accordance with Michaelis-Menten kinetics and the Hill generalized function method [6], Fick's diffusion law and the mass action law (to describe active transport). Alternatively, users can create their own functions instead of the default ones. The parameters_fitting.m file describes the implementation of a genetic algorithm for assessing the similarity of the simulated distribution to experimental data. The model_parameters.m file contains all the model parameter default values for the ODE system and describes the model configuration (substance inflows). The grow_eq.m file describes the cell growth function, and tool_1d_model.m file provides the modeling scenario. It is important to note that there are two different strategies for using DyCeModel: using the parameters_fitting.m file or

not using it. In the latter case, the user should define all parameters in the `model_parameters.m` file.

Results: The DyCeModel tool builds mathematical models of hormone distribution based on the processes of their synthesis, degradation, diffusion and active transport in a dynamically developing cellular ensemble. As DyCeModel allows to model different types of plant meristems based on the same ODEs with a set of certain input characteristics for different meristems, we demonstrated the effectiveness of the tool by modeling the influence of main plant hormones auxin and cytokinin on tissue patterning in two types of *Arabidopsis thaliana* stem cell niches: root and shoot apical meristems. Using DyCeModel, we built the models of the root and shoot apical meristems by automatically selecting model parameters that matched the experimental data. For automatically parameters fitting we used the following restrictions on parameter values: approximately equal values of diffusion parameters for auxin and cytokinin and a low level of auxin synthesis. Obtained hormone distribution profiles in the models were qualitatively consistent with published experimental data. In result, proliferative activity zones were identified and the number of cells within those zones were maintained at a certain level throughout the entire time of model calculations. At the same time, the identified parameters of passive transport, degradation and growth were the same for the shoot meristem and root meristem models, and the parameters determining cell division remained similar.

Conclusion: The developed DyCeModel tool is quite flexible; it provides embedding, addition, and mixing of existing mathematical models. If you have experimental data of interest substance, it is possible to automatically select unknown parameters, which speeds up work with the model and makes it more stable. As an output, DyCeModel produces a statistical summary of cellular composition that can be used to predict the effect of hormones on cell proliferation activity. The resulting models provide a promising framework for further study of the role of hormone-controlled gene regulatory networks in cell dynamics.

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