Preface

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Historically, mathematical models have been essential to understand plant physiology [12]. They provided rules that could be applied to predict crop growth and yield in the field, made farm management more efficient and helped to increase productivity. For example, the 'law of minimum' proposed by Liebig in 1840, states that crop yield is limited by the availability of a most deficient nutrient. Farmers would then simply need to identify requirements for each nutrient in order to obtain optimal yield. Liebig's law formalised plant requirements in a simple and quantitative fashion and allowed generations of farmers to optimise the application of fertilisers. Unfortunately, complex biological functions of plants cannot be described as a superposition of independent environmental effects in the way Liebig described plant nutrition. Plants possess complex self-organised molecular machineries and exhibit a wide range of responses. For example, sensing proteins in root apical meristems are involved in the detection of nutrients and cascades of signals are triggered to stimulate lateral root proliferation in nutrient patches [13, 21]. Although shoot architectures follow more predictable growth patterns, e.g. phyllotactic arrangement of leaves, they also arise from multiple interactions and feedbacks between cells, tissues and organs [24]. Flowering time in a plant, for example, results from subtle interactions between circadian clock genes regulating day-night sensing and the physiology of photosynthesis and carbon allocation [8].

Early computational biologists understood the limitations of classical agronomic and physiological modelling and initiated alternative approaches. Lindenmayer, a botanist interested in growth patterns of algae and trees, proposed in 1968 a framework named 'L-systems' to formalise rules for the development of plant architectures [30]. It became possible to model interactions between plant architecture and the environment, a concept now termed 'Functional Structural Plant Models' [14, 16]. In 1969 Korn also noticed that since plant growth and functions are determined by individual cells, the cellular structures of a tissue must be incorporated [25]. In his first model, Korn described the development of a plant tissue from a simple stochastic cell cycle model. The field of plant modelling has grown considerably over the last decades and the concepts of Korn and Lindenmayer evolved. Architectural models now incorporate plant physiology explicitly and are combined with models of the environment to account for, e.g. nutrient transport in soil and light interception [7, 9]. New computational cellular models are able to simulate thousands of cells [34], and include autonomous genetic regulatory networks, the sensing and response to hormonal signals as well as turgor pressure driven expansion [10, 20]. Modelling languages such as the 'Systems Biology Markup Language' have been developed to model metabolic pathways [31].

Because plants are immobile they must be able to sense their environment and adapt to numerous external cues. Responses to environmental signals are actioned at the cell level, where biological processes are broken down into chains and networks of biochemical reactions. Long range signals between cells are also required to coordinate activities. Signalling molecules, named hormones, are produced and

transported across tissues to promote different cellular activities, such as proliferation or differentiation. The work presented by Muraro, Byrne, King & Bennett on "*Mathematical modelling of plant signalling networks*" provides an overview of different approaches available to model signalling networks in plant cells. Popular deterministic models of regulatory processes include Boolean networks and systems of ordinary differential equations. Gene expression is highly stochastic, and use of stochastic reaction kinetics and Bayesian network models have become essential to model low concentration reactions and infer biochemical networks from data. More recent developments include a better representation of the multicellular nature of signalling and regulatory networks.

Though plant cell expansion and differentiation is genetically regulated, it is constrained physically by cell walls and membranes. Plant growth may be represented as a balance between forces acting on cell walls due to turgor pressure and/or external loads, and stresses in cell walls created by the deformation. The first model of irreversible cell expansion was described by Lockhart in 1965 by relating the strain rate to the turgor pressure via a cell wall extensibility and a yield threshold [27]. Since then, many generalisations have been proposed. For example, rates of transpiration and elastic deformation were introduced into Lockhart's model to account for these effects [15]. The microstructure of the cell wall has been considered by distinguishing between the free energies related to either the elasticity of macromolecules and of hydrogen bonds [36], or to the matrix and microfibril phases of the wall [4]. The influence of the elastic properties of the wall matrix, the cellulose microfibrils' orientation and the external torque on the expansion process has been analysed by modelling the cell wall as a fibre-reinforced viscous fluid [11]. The widely used 'decomposition approach' of a deformation tensor into elastic and growth part has also been applied to model the growth of cell walls [23], and anisotropic tissue growth [17]. Clearly, the diversity of models is very high. Ortega & Welch review in "*Mathematical models for expansive growth of cells with walls*" a wide spectrum of mechanical models of cell and tissue growth.

The homeostasis and control of growth is an important question in modelling and understanding plant development. Pollen tubes have been subject of extensive theoretical research, among many others [5,18,26,32], due to their rich structure and being well accessible to *in vitro* experiments. It was observed that the growth of pollen tubes oscillates in time and that the fluxes of some ions, such as calcium, follow this behaviour [29]. This gives rise to the questions of how growth is exactly regulated, and if the oscillations are harmonic and describable by well-known physical models of harmonically oscillating systems. In order to answer this question it is necessary to study changes in the oscillation frequency, amplitude and phase resetting under permanent or temporary changes of growth conditions, such as variable extracellular pH, borate and calcium concentration or application of pectin methyl esterase [6]. The studies in "*Pollen tubes with more viscous cell walls oscillate at lower frequencies*" by Kroeger & Geitmann investigate further the nature of pollen tube growth oscillations. The authors show that these are not harmonic, non-isochronous and the period of oscillation depends on their amplitudes. To analyse the experimentally known reduction of average growth rate of pollen tubes upon application of extracellular calcium or borate, the well-known Lockhart growth model was generalised by considering a time-dependent cell wall viscosity. For the dynamics of the cell wall viscosity, it was assumed that the changes in viscosity are inversely proportional to the cytosolic calcium concentration. Borate is thought to modify rheological properties of pectin, a major component of the pollen tube cell wall. The influence of borate on the growth dynamics was addressed by changing the value of the maximal density of bonds between pectin monomers during the growth cycle, given as a parameter in the equation for the cell wall viscosity.

In order to understand plant development, it is essential to use the cell as the main modelling unit. Growth is then represented as a sequence of cell division, expansion and differentiation, of which the direction and magnitude contribute to the formation of organs [3]. The coupling between elastic deformation of plant cell walls, growth and internal biochemical processes was considered in "*Deformable cell model and its application to growth of plant meristems*" by Bessenov, Mironova & Volpert. The developed elastic model distinguishes between expanding, growing and dividing, as well as only deforming cells. An individual cell at the equilibrium was represented as a regular polygon with a number of

vertices, connected by springs, and a particle of certain mass in each vertex. Three forces acting on the vertices and depending on the changes of side length, angle and volume were considered to define the elastic deformations. It was shown that the direction of cell division is crucial for the properties of growing cell structures. One of the important features of plants is the formation of self-similar structures which reproduce the same cell organisation during development. The precise choice of mechanical properties of cell walls ensures the existence of self-similar solutions of the considered elastic growth model. The growth hormone auxin is essential for the regulation of growth. To analyse the dynamics of auxin in a plant organ its diffusion and polar transport were introduced into the model.

Along with biomechanical processes, the uptake of water and nutrients by plant roots and their transport through plant organs are essential for proper development. Transport proteins are required for the movement of solutes through membranes, which represent the interface between symplast and apoplast [19]. A first model of water transport in plants, describing the flow in analogy to an electric current through a resistor network, was presumably the one proposed by van den Honert [22,35]. Pressure assumes in that approach the role of the electric potential and the flux of water is given by the product of the hydraulic conductivity and the pressure gradient. Later, this pressure driven flux was extended to include osmotically driven fluxes (diffusional fluxes) and the concept of water potential was introduced [28]. Along with models of solute transport around roots and uptake on the root surface [33], the description of the movement of water and solutes inside a root tissue or organ requires new modelling approaches, which include a precise description of the interaction of the symplast and apoplast. A multiscale model for water and solute transport in a plant tissue was developed in "*Homogenization approach to water transport in plant tissues with periodic microstructures*" by CHAVARRÍA-KRAUSER & PTASHNYK. The model considers the microscopic structure of a plant cell comprising continua of symplast and apoplast. The derived transmission conditions at the cell–membrane–cell wall interface reflect the osmotic nature of water flow through semipermeable membranes. Transport of the solute was allowed to take place opposite to the gradient of chemical potential by means of surface reactions. The authors derived a macroscopic model for fluid flow and transport of osmotically active solutes using multiscale analysis. The macroscopic flow velocity follows a Darcy law with a force term, where the driving force is given by the local difference of symplastic and apoplastic solute concentrations.

The development of computational methodological modelling frameworks provides easy implementation of analytic approaches to study aspects of complex biological systems. The software platform presented in "*Development and Evaluation of Plant Growth Models: Methodology and Implementation in the PYGMALION platform*" by COURNÉDE, CHEN, WU, BAEY & BAYOL aims exactly at providing such a modelling framework. PYGMALION (Plant growth model analysis, identification and optimisation) purposes at providing an easy implementation of discrete in time Markovian models describing different compartments of a plant. The platform was developed in C++ and evaluation of a model, sensitivity analysis and parameter estimation are the main tools incorporated in the software. To account for the uncertainty and to provide sensitivity analysis for inputs of the models, the regression coefficients method, Sobolev's variance-based method and Morris's method were implemented. Frequentist and Bayesian approaches were included in the platform for estimation of parameters. Classical models and a new Log Normal Allocation and Senescence model for sugar beet growth comprising foliage and root compartments were implemented in PYGMALION and presented in the manuscript.

The world agriculture is now under numerous new pressures. The global population is rising, climate change will produce more droughts and extreme weather, the fertility of soil is declining, water is becoming more scarce and the cost of fertilisers is increasing. Reliable plant models are required to address these challenges. They could assist land management, so that all field inputs are in response to weather and soil data, and crop yield is maximised based on model predictions [1]. Models could also be used to identify traits that make crops better adapted to future environmental conditions [2]. Unfortunately, current models are not able to predict reliably the responses to changes in environmental conditions, as plants are extremely adaptable organisms. A new generation of plant models must be developed to better predict plant growth responses. Processes of various types and at different scales, from a single cell to the

entire organism, will be required to communicate between themselves and interact with the environment. This special issue demonstrates that numerous modelling concepts exist. It is now the time to unify these concepts and propose generic frameworks to face the upcoming challenges of agriculture.

References

[1] B. Basso, J.T. Ritchie, F.J. Pierce, R.P. Braga, J.W. Jones. *Spatial validation of crop models for precision agriculture.* Agr. Syst., 68 (2001), 97–112.

[2] L.K. Brown, T.S. George, L.X. Dupuy, P.J. White. *A conceptual model of root hair ideotypes for future agricultural environments: what combination of traits should be targeted to cope with limited P availability?* Ann. Bot., (2012), 1–14.

[3] V. Brukhin, N. Morozova. *Plant growth and development – Basic knowledge and current views.* Math. Model. Nat. Phenom., 6 (2011), 1–53.

[4] M.A.J. Chaplain. *The Strain Energy Function of an Ideal Plant Cell Wall.* J. Theor. Biol., 163 (1993), 77–97.

[5] A. Chavarría-Krauser, D.Yejie. *A model of plasma membrane flow and cytosis regulation in growing pollen tubes.* J. Theor. Biol., 285 (2011), 10–24.

[6] Y. Chebli, A. Geitmann. *Mechanical principles governing pollen tube growth.* Func. Plant Sci. Biotech., 1 (2007), 232–245.

[7] M. Chelle. *Phylloclimate or the climate perceived by individual plant organs: What is it? How to model it? What for?.* New Phytol., 166 (2005), 781–790.

[8] Y. H. Chew, A.M. Wilczek, M. Williams, S.M. Welch, J. Schmitt, K.J. Halliday. *An augmented Arabidopsis phenology model reveals seasonal temperature control of flowering time.* New Phytol., 194 (2012), 654–665.

[9] X. Draye, Y. Kim, G. Lobet, M. Javaux. *Model-assisted integration of physiological and environmental constraints affecting the dynamic and spatial patterns of root water uptake from soils.* J. Exp. Bot. 61 (2010), 2145–2155.

[10] L.X. Dupuy, J. Mackenzie, J. Haseloff. *Regulation of plant cell division in a simple morphogenetic system.* P. Natl. Acad. Sci. USA, 107 (2010), 2711–2716.

[11] R.J. Dyson, O.E. Jensen. *A fibre-reinforced fluid model of anisotropic plant cell growth.* J. Fluid Mech., 655 (2010), 474–503.

[12] M.A. El-Sharkawy. *Overview: early history of crop growth and photosynthesis modeling.* BioSystems, 103 (2011), 205–211.

[13] B.G. Forde, P.I.A. Walch-Liu. *Nitrate and glutamate as environmental cues for behavioural responses in plant roots.* Plant Cell Environ., 32 (2009), 682–693.

[14] T. Fourcaud, X. Zhang, A. Stokes, H. Lambers, C. Körner *Plant Growth Modelling and Applications: The Increasing Importance of Plant Architecture in Growth Models.* Ann. Bot., 101 (2008), 1053–1063.

[15] A. Geitmann, J.K.E. Ortega. *Mechanics and modeling of plant cell growth.* Trends Plant Sci., 14 (2009), 467–478.

[16] C. Godin, H. Sinoquet. *Functional-structural plant modelling.* New Phytol., 166 (2005), 705–708.

[17] A. Goriely, D.E. Moulton, R. Vandiver. *Elastic cavitation, tube hollowing, and differential growth in plants and biological tissues.* EPL-EuroPhys. Lett., 91 (2010), 18001.

[18] A. Goriely, M. Tabor. *Mathematical modeling of hyphal tip growth.* Fungal Biol. Rev., (2008), 1–7.

[19] J.L. Hall, L.E. Williams. *Transition metal transporters in plants.* J. Exp. Bot., 54 (2003), 2601–2613.

[20] M.G. Heisler, H. Jönsson. *Modelling meristem development in plants.* Curr. Opin. Plant Biol., 10 (2007), 92–97.

[21] A. Hodge. *Root decisions.* Plant Cell Environ., 32 (2009), 628–640.

[22] T.H. van den Honert. *Water transport in plants as a catenary process.* Discuss. Faraday Soc., 3 (1948), 146–153.

[23] R. Huang, A.A. Becker, I.A. Jones. *Modelling cell wall growth using a fibre-reinforced hyperelastic-viscoplastic constitutive law.* J. Mech. Phys. Sol., 60 (2012), 750–783.

[24] H. Jönsson, M.G. Heisler, B.E. Shapiro, E.M. Meyerowitz, Mjolsness E. *An auxin-driven polarized transport model for phyllotaxis.* P. Nat. Acad. Sci. USA, 103 (2006), 1633–1638.

[25] R.W. Korn. *A stochastic approach to the development of Coleocheate.* J. Theor. Biol., 24 (1969), 147–158.

[26] J.H. Kroeger, R. Zerzour, A. Geitman. *Regulator or Driving Force? The Role of Turgor Pressure in Oscillatory Plant Cell Growth.* PLoS One, 6 (2011), e18549.

[27] J.A. Lockhart. *An analysis of irreversible plant cell elongation.* J. Theor. Biol., 8 (1965), 264–275.

[28] P. Nobel. *Physicochemical & Environmental Plant Physiology.* Academic Press, 1999.

[29] E.S. Pierson, D.D. Miller, D.A. Callaham, J. van Aken, G. Hackett, P.K. Hepler. *Tip-Localized Calcium Entry Fluctuates during Pollen Tube Growth.* Dev. Biol., 174 (1996), 160–173.

[30] P. Prusinkiewicz, A. Lindenmayer. *The Algorithmic Beauty of Plants.* Springer, 1991.

[31] J.M. Rohwer. *Kinetic modelling of plant metabolic pathways.* J. Exp. Bot., 63 (2012), 2275–2292.

[32] E.R. Rojas, S. Hotton, J. Dumais. *Chemically Mediated Mechanical Expansion of the Pollen Tube Cell Wall.* Biophys. J., 101 (2011), 1844–1853.

[33] T. Roose, A. Schnepf. *Mathematical models of plant-soil interaction.* Phil. Trans. Royal Soc. A, 366 (2008), 4597–4611.

[34] T.J. Rudge, P.J. Steiner, A. Phillips, J. Haseloff. *Computational modeling of synthetic microbial biofilms.* ACS Synth. Biol., 1 (2012), 345–352.

[35] M.T. Tyree. *The Cohension-Tension theory of sap ascent: current controversies.* J. Exp. Bot., 48 (1997), 1753–1765.

[36] B.A. Veytsman, D.J. Cosgrove. *A Model of Cell Wall Expansion Based on Thermodynamics of Polymer Networks.* Biophys. J., 75 (1998), 2240–2250.