IJPB Symposium 2024

Plant Modeling: Opportunities and Challenges

Versailles, France, 13-15 May 2024

Abstract Book

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Brief introduction

The **Institute Jean-Pierre Bourgin for Plant Sciences**, a major laboratory for plant science research affiliated to **INRAE** and **AgroParisTech** and part of **Paris-Saclay University**, is organising in 2024 the second edition of its international symposium.
Following on the first edition in 2018, this event takes place from the 13th to 15th of May 2024 at the INRAE Centre in Versailles.

The 2024 edition is dedicated to **plant modeling**, a groundbreaking research strategy adopted by the IJPB to better understand the complexity of plant biology.

The symposium comprises three plenary conferences and four thematic sessions dealing with modeling at different scales, from the intra-cellular to the macroscopic level. The aim of this exciting meeting is to foster collaborations and facilitate knowledge exchange among participants by bringing together renowned specialists in the field.
The symposium also features **workshops on microscopy and imaging**, conducted in collaboration with the imaging and microscopy platform (PO-Cyto) of the Plant Observatory (OV) and the "Modeling and Digital Imaging" (MIN) and "Primary Cell Wall" (PAR) teams of the IJPB.

This forward-looking symposium provides a unique opportunity to evaluate recent advances in modeling, explore how it can be integrated experimentally, and examine how it adapts to the constant increase in computing power and the explosion of data.

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Many thanks to all the IJPB members who helped and supported us continuously throughout the organization of this event.
Many thanks to the INRAE Île-de-France – Versailles-Saclay Research Center for making their facilities available and helping us to organize this event.

Thanks to our sponsors

The organization of the symposium would not have been possible without the help of our sponsors, and we sincerely thank them for their financial support.

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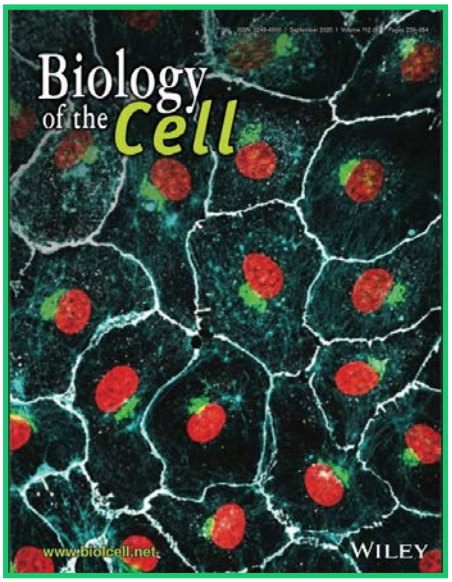

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Program Overview

Monday, May 13th

12:30 - 13:50 Registration
13:50 - 14:10 Welcoming

14:10 - 15:10 Keynote speaker: Manuel Théry
Morphogenesis by microtubule networks
Chair: Samantha Vernhettes, Magalie Uyttewaal

15:10 - 16:30 Session 1: Modeling plant biomass

Chair: Stéphanie Baumberger, Matthieu Reymond, Adithya Raveendran Thottathil

15:10 - 15:50 Sofiane Guessasma
Modeling of the mechanical behaviour of plant fibres from synchrotron radiation data: Towards a better understanding of the ultrastructure effect for engineering applications
15:50 - 16:10 Solmaz Hossein Khani
4D Characterization of Plant Cell Wall Enzymatic Hydrolysis in Highly Deconstructed Samples
16:10 - 16:30 Marco d'Agostino
Modeling plant water uptake: from cross sections to root architecture
16:30 - 17:00 Coffee break
17:00 - 17:40 Yassin Refahi
4D Analysis and Modelling of Plant Cell Wall Deconstruction
17:40 - 18:00 Yasmeen Hitti
Network Analysis for Plant Extracellular Signals
18:00 - 18:20 Edgar Steven Correa Pinzon
Drought stress Patterns recognition in Rainfed Rice: Senegal study case

18:20 - 18:40 Poster flash talks

18:40 - 20:00 Poster session & Coktail event at IJPB

Tuesday, May 14th

09:00 - 11:00 Session 2: Genes & metabolism

Chair: Nicolas Arnaud, Massimiliano Corso, Léa Barreda.

09:00 - 09:40 Rea Laila Antoniou-Kourounioti
Modelling environmental and epigenetic regulation of flowering time
09:40 - 10:20 Olivier Loudet & **Anne Goelzer**
Arabidopsis natural variation reveals complex GxE interactions: we need an 'RBA' model!
10:20 - 10:40 Gilles Curien
ChloroKB web application and The Arabidopsis Leaf Quantitative Atlas: tools for modelling plant metabolism
10:40 - 11:00 Anze Zupanic
SKM and Booldog - From knowledge graph to dynamic Boolean modelling
11:00 - 11:30 Coffee break
11:30 - 12:10 Pierre Petriacq
Metabolome modelling to decipher plant performance
12:10 - 12:30 Amy Briffa

Is the variation of intragenic DNA methylation in Arabidopsis natural populations governed by genetic or epigenetic inheritance?

12:30 - 12:50 Jan Zrimec

Modelling potato primary and secondary metabolism captures the principles of plant growth and defence under biotic stress

12:50 - 13:00 Private company presentations

13:00 - 14:00 Lunch break

14:00 - 16:30 Workshops & visits of IJPB infrastructures

16:30 - 17:00 Coffee Break

17:00 - 18:00 Keynote Speaker: Philippe Andrey

Image-based modeling of cell division patterns

Chair: Magalie Uyttewaal, Samantha Vernhettes

18:00 - 19:00 Keynote Speaker: Adrienne Roeder

Robustness in the morphogenesis of Arabidopsis sepals

Chair: Magalie Uyttewaal, Samantha Vernhettes

19:00 - 23:00 Social event: Ferme du prieuré

Wednesday, May 15

09:00 - 11:00 Session 3: Cell, tissue, development

Chair: Magalie Uyttewaal, Samantha Vernhettes, Luka Lelas.

09:00 - 09:40 Pau Formosa-Jordan

Multicellular dynamics of plant growing tissues - integrating quantitative imaging and modelling

09:40 - 10:20 Kalina Haas

Data Collection Challenges for Integrative Modeling of Plant Cell Growth: Insights from Super-Resolution and Time-Lapse Microscopy

10:20 - 10:40 Jeanne Abitbol-Spangaro

Plasmodesmata-mediated diffusion is a sufficient transport mechanism for generating the auxin gradients regulating branch patterning in a moss leafy shoot

10:40 - 11:00 Laure Mancini

Control of the spiral phyllotaxis from a single stem cell in the moss Physcomitrium patens

11:00 - 11:30 Coffee break

11:30 - 12:10 Kirsten ten Tusscher

Multi-scale modeling of root system growth and patterning

12:10 - 12:30 Marie Zilliox

Finding the determinants of various 3D growth strategies in brown algae

12:30 - 12:50 Elsa Gascon

Numerical reconstruction of plants seeds for morphogenesis analysis

12:50 - 14:00 Lunch break

14:00 - 16:00 Session 4: Integration across scales and modalities

*Chair: Philippe Andrey, Loïc Rajjou, Sophie Bigo***t**.

14:00 - 14:40 Wolfram Weckwerth

Genomic prediction and analysis of causal relations in metabolic networks of plant germplasm collections combining multivariate statistics and AI

14:40 - 15:20 Jasmine Burguet

Quantification and modeling of leaf morphogenesis

15:20 - 15:40 David Legland

Morphometry and growth of wheat grain by registration of 3D tomography image

15:40 - 16:10 Coffee break

16:10 - 16:50 Krzysztof Wabnik

Towards mechano-biochemical computer models of plant development

16:50 - 17:10 Isabelle Fobis-Loisy

Geometric and mechanical guidance: role of stigmatic epidermis in early pollen tube pathfinding in Arabidopsis

17:10 - 17:30 Ray Ratula

Modeling ovule curvature

17:30 - 17:40 Closing & announcements

Abstracts

Plasmodesmata-mediated diffusion is a sufficient mechanism for generating the auxin gradients regulating branch patterning in a moss leafy shoot

Jeanne Abitbol-Spangaro[1], Yoan Coudert[1], Christophe Godin[1]

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Land plants have evolved a great diversity of branching architectures, yet questions persist regarding the mechanisms driving their emergence during plant development. In flowering plants, shoot apical meristems control plant architecture by inhibiting new branch initiation at a distance, through the action of the phytohormone auxin. Auxin synthesized in apices undergoes active transport from cell-to-cell through polar membrane transporters, generating a basipetal bulk auxin flow. Despite the evolutionary divergence of mosses from flowering plants several hundred million years ago, they exhibit similar auxin-dependent branching control (Coudert, 2015; Thelander, 2022). However, in the moss Physcomitrium patens, a regulatory mechanism based on polar auxin transport cannot explain the branching patterns. Moreover, PIN proteins have a minor role in shoot branching control. Experimental data suggest that the symplasmic pathway, *i.e.* plasmodesmata-mediated diffusion, could instead represent the main route for auxin movement in the stem. However, flowering plant studies have shown that although plasmodesmata are involved in conveying molecules in multiple developmental processes, their contribution is often limited or localized. Indeed, diffusion is a slow transport mechanism that loses efficiency over distance. In this context, my work aims at testing the hypothesis that symplasmic auxin diffusion can generate the auxin gradients necessary for branching control in moss at the whole shoot level. To this end, I collected biological data related to cell geometry and plasmodesmata distribution and developed a computational model of auxin symplasmic diffusion in an idealized three-dimensional moss shoot. This integrative and quantitative approach enables me to demonstrate that a regulatory mechanism based on plasmodesmata-mediated auxin diffusion can account for branching patterns observed in real shoots.

References

1. Coudert, Y. *et al.* Three ancient hormonal cues co-ordinate shoot branching in a moss. *eLife* **4**, e06808 (2015).

2. Thelander, M. *et al.* Apical dominance control by TAR-YUC-mediated auxin biosynthesis is a deep homology of land plants. *Current Biology* **32**, 3838-3846.e5 (2022).

Morphogenetic determinants of plant female germ cell precursors specification and plasticity

Inès Ouedraogo[1], Gabriella Mosca[2], Elvira Hernandez-Lagana[1], Ethel Mendocila-Sato[3], Luciana Delgado[4], Olivier Leblanc[1], Geneviève Conéjéro[5,6], Célia Baroux[3], Daphné Autran[1]

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[4] Instituto de Investigaciones en Ciencias Agrarias de Rosario (IICAR), CONICET, University of Rosario, Argentina,
[5] Research Unit AGAP Institute, CIRAD, INRAE, Institut Agro, University of Montpellier, France,
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In higher plants, female gametes formation is a crucial step in the plant reproductive cycle and determines seed formation, hence participating in crop yields. The plant female germline initiates in the ovule primordium, with the specification of the Megaspore Mother Cell (MMC), the only cell which will undergo meiosis to produce gametes. However, germ cell fate in the early ovule appears plastic. Genetic variants and apomictic species show that somatic cells neighboring the MMC can enter the MMC identity program or even directly produce female gametophytes without meiosis. By combining 3D morphometrics, growth modelling, gene markers and genetic analyses, we have shown in Arabidopsis that this developmental plasticity is also part of MMC ontology in wild-type, before channeling toward MMC singleness, a process controlled by ovule tissue growth. Recently, we developed new routes further exploring Arabidopsis MMC growth using time-lapse (3D+t), and establishing a 3D morphometric atlas of ovule primordia in Maize, a sexual grass model, to understand the genericity of MMC formation and its plasticity.

Automated quantitative morphological analysis of intracellular structures: application to the mitotic spindle of *Arabidopsis thaliana* root tip

Martine Pastuglia, Jasmine Burguet, Katia Belcram

Institut Jean-Pierre Bourgin (IJPB - INRAE ˆIle-de-France - Versailles-Saclay) – Institut National de la Recherche Agronomique - INRA (FRANCE) – Route de Saint-Cyr 78026 Versailles cedex, France

Bipolar spindles ensure equal distribution of chromosomes during mitosis. In plant, spindles are acentrosomal with microtubules converged toward broad, diffuse poles. Plant cell spindles exhibit great plasticity in their morphology and size depending on the cell type but published works, up to now, are restricted to 2D measures. Here we have developed an analysis pipeline to measure spindle and cell shape in 3D. Our model is the Arabidopsis root meristem, a zone of active divisions located at the root tip and composed of several cell types that differ in size and shape. The analysis requires 3D confocal stacks of Arabidopsis roots immuno-localized with an antitubulin antibody (for spindle labeling), and double-stained with a nucleus (for metaphase plate labeling) and a cell wall dye (allowing segmentation of cells). Each metaphase cell is segmented, then the pipeline automatically extracts the cell's and spindle's shape parameters enabling a precise measurement of spindle size and morphology within the cell (spindle and cell length, width, volume, etc…). We will present the first data obtained using this pipeline in a wild-type background. Our results indicates that in 3D, spindles from all different cell types tend to be radially symmetric even if the cell shape is not. We also confirm that each cell type has a distinct spindle geometry. Within a particular cell type, the spindle volume stays constant, even when the cell volume enlarges. We are now using mutants affecting cell shape to determine to what extent spindle morphology is determined by cell geometry rather than by genetic and developmental programs expressed in each cell. We also plan to analyze mutation mildly affecting spindle shape to evaluate the sensitivity of this new procedure to detect spindle defects.

Spatiotemporal gene expression models reveal the Arabidopsis leaf gene regulatory network topology

Sophie Bigot[1], Jasmine Burguet[1*] and Nicolas Arnaud[1*]

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*Equal contribution

Plant development is a highly dynamic process, which relies on the coordinated action of gene products. Further, gene expression is tightly regulated both in space and in time to ensure the development of reproducible organs. Expression patterns of key regulators are often only qualitatively characterized. So far, quantitative information about their temporal dynamics, the genetic determinants of their spatial expression, the links between them and feedbacks with tissue growth are often lacking. To face this complexity, we developed a method to spatially average expression pattern in 2D onto a common developing organ scaffold model. Applied to the analysis of leaf growth, this allowed us to access the spatiotemporal dynamics of gene expression patterns in relation with changing organ morphology. As related expression dynamics may indicate direct network connectivity, we infer regulatory interactions within the CUP-SHAPED COTYLEDON 2 (CUC2) centered network. CUC2 is a key transcription factor involved in both patterning and growth at the leaf margin. Using our methodology, we predict CUC2 primary and secondary targets before validating the predicted interactions *in vivo*. This work provides valuable information about the CUC gene regulatory network and highlights that expression patterns can be used as quantitative objects to reliably predict network topology.

BIP, a new software for reproducible batch processing of biological images

Eric Biot [1], Sandrine Lefranc[1], Ayoub Ouddah[1], Jasmine Burguet[1], Philippe Andrey[1]

[1] *Université Paris-Saclay, INRAE, AgroParisTech, Institut Jean-Pierre Bourgin (IJPB), 78000, Versailles, France*

Biological imaging is one of the main tools used by biologists to decipher how plants function. Extracting quantitative information from microscopy images typically requires complex image processing and analysis pipelines combining elementary operations such as signal enhancement, object segmentation and object measurements. In addition, data integration through the processing of large image sets is necessary to model variability and ensure robust analysis. Image analysis software fall into two categories. On the one hand, specialised libraries such as ITK provide collections of basic components that can be assembled into potentially complex image processing sequences, but require a high level of computer programming expertise. On the other hand, integrated software such as Fiji provides user-friendly graphical interfaces that allow end-users with little or no programming knowledge to perform a wide range of pre-defined image processing operations. However, automation and batch processing capabilities are often limited and do not eliminate the need for user programming.

We address these limitations by proposing a new software, for reproducible batch processing and analysis of biological images. BIP integrates many standard algorithms and specific algorithms developed in our research projects for quantifying images of plant cells and tissues. BIP fills an empty niche in the bioimaging software ecosystem by relying on a simple yet powerful command-line interface that can be used from individual workstations to HPC solutions. With BIP, users easily specify sets of images for processing and readily chain basic operations into complex analysis pipelines. BIP offers transparent support for images of arbitrary dimensions (2D to 5D) and numerical types (integers and floats, signed and unsigned, from 8 to 64 bits), eliminating the compatibility barriers often encountered in existing software, thanks to a unified data structure for representing multi-dimensional images and a generic design pattern for the automatic detection of numerical data types. In addition, these design principles minimize the work involved in implementing each algorithm, facilitating code maintenance, evolution and optimization. Here, we illustrate through several examples the benefits and potential of BIP for processing and quantifying image datasets of plant cells and tissues, including 3D time-lapse confocal images of *A. thaliana* shoot apical meristems.

Is the variation of intragenic DNA methylation in Arabidopsis natural populations governed by genetic or epigenetic inheritance?

Amy Briffa[1#], Elizabeth Hollwey[2,3#], Jonathan D. Moore[2], David B. Lyons[2], Zaigham Shahzad[2,4], Martin Howard[1*], Daniel Zilberman[2,3*]

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Gene body methylation (gbM) in plants shows stable transgenerational inheritance, despite the imperfect fidelity of semiconservative maintenance by MET1/Dnmt1. The model organism Arabidopsis is an ideal system to study these fundamental CG methylation (mG) dynamics at both short and evolutionary timescales. It is an open question whether the mCG variation seen in natural populations is governed by genetic or epigenetic inheritance. Computational modelling provides an essential tool to uncouple these two components, while providing access to experimentally inaccessible timescales.

Through an integrated experimental and computational approach, we find substantial *de novo* activity, which is strongly enhanced by existing proximate methylation (i.e. cooperative non-linear feedback). This cooperative de novo MET1 activity both seeds and stably propagates gbM, demonstrating that intragenic mCG establishment and inheritance constitute a unified epigenetic process. Our mathematical model precisely reproduces the spatial mCG inheritance dynamics, predicting the observed steady-state mCG patterns, such as mCG enrichment over CG-site dense exons, from zero initial methylation (i.e. given only the CG site spacing within methylatable regions as input).

Remarkably, even in the absence of any selection pressure, this simple stochastic model of purely epigenetic inheritance can explain the majority of the observed population-scale variation, providing strong evidence that gbM is a stochastic phenomenon. While steady-state gbM levels are genetically determined, we find that the methylation level at any given time undergoes substantial continuous epigenetic fluctuations on millennia-long timescales. Gene body methylation in plants is thus an archetype of long-term stable transgenerational epigenetic inheritance with the potential to mediate evolution. Much recent attention has focussed on the imminent loss of genetic biodiversity. Our results raise the question of whether there may be a hitherto unappreciated epigenetic component also at risk.

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Spatial statistics to model the 3D organization of point-cloud patterns in finite domains

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Functions and spatial architectures are tightly linked in biological systems. Imaging techniques such as confocal microscopy can reveal how biological structures are organized in 3D, and how they may differ depending on, e.g., genetic lines or experimental condition. Repeated acquisitions also provide access to spatial variability. Adapted statistical tools for the quantitative analysis and comparison of spatial organizations from sets of digital images are required. Here we focus on biological structures appearing as point patterns in 3D and distributed over finite domains (e.g., vesicles in cells or neurons in brains). This point-cloud nature makes spatial analysis difficult: the number and positions of single points typically vary between different instances of the same domain (cell, brain…), which are also subject to shape variability. To face this complexity, we propose a point intensity mapping strategy within a standardized spatial domain. Given a sample of n point sets within the n corresponding domains (e.g., 3D positions of a given endosome population labeled within n cells), we assume the existence of a common underlying point process that generated this sample. To reconstruct this process, we estimate its point intensity variations. After a normalization procedure that projects all point sets within an average 3D domain, our strategy is based on a local statistical estimator of point intensity that relies on distances to k-th nearest neighbors. A method for efficiently correcting the border estimation bias is also proposed. The statistical comparison of two distributions (e.g., those of endosomes labeled in two different conditions) can then be mapped in space by repeating local intensity comparisons, thus highlighting regions with significant intensity differences. This global strategy should significantly contribute to the quantitative deciphering of complex biological systems.

Towards the modeling of chromosome movements during meiotic prophase I in *Arabidopsis thaliana*

Anca Caranfil[1], Laurence Cromer[1], Sandrine Lefranc[1], Mathilde Grelon[1], Philippe Andrey[1]

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During meiotic prophase I, chromosomes undergo rapid prophase movements and change their configuration in the nucleus. Studies in yeast showed that these movements play an important role in achieving non-erroneous meiosis, but little is known about this mechanism in plants. Using advanced imaging techniques and quantitative image analysis, we have recently brought to light a similar behavior in *Arabidopsis thaliana*. One aspect to decipher now is what causes these movements, and how they are affected by physical constraints inside the cell nucleus. We propose to address this question by modeling chromosome movements using polymer physics and molecular dynamics simulations. Our model takes into account several topological constraints specific to meiosis, such as the attachment of the telomeres to the nuclear envelope or the external cytoskeleton forces that act on the telomeres. We report here preliminary results obtained with this model and study how geometrical and topological constraints affect chromosome dynamics and can promote or impede their movements. Combining this model with experimental data will provide the means to better understand the behavior observed in movement-disruptive mutants in *Arabidopsis thaliana*.

Drought stress Patterns recognition in Rainfed Rice: Senegal study case

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The interaction among rice cultivar types, environmental factors, and agronomic practices is crucial for determining crop yield. This research involves the characterization of drought stress through in-silico simulations using the mechanistic crop model DSSAT in the Casamance region of Senegal.
Drought is one of the most limiting factors in rice production, poses a substantial obstacle in rice cultivation, impacting growth, yield, and grain quality [1][2]. The gravity of this limitation is exacerbated by fluctuations in climate patterns and constraints on water resources [3]. Mitigating these challenges necessitates the integration of drought-tolerant rice cultivars and effective agricultural management strategies [4].

This research hypothesizes that mechanistic crop models assisting in identifying drought stress patterns across entire regions for rainfed rice cultivation in Senegal. The first phase of the research involves calibrating and validating the crop model using error metrics such as R2, RMSE, and Efficacy. In the second phase, in-silico simulations are conducted to establish the target population of environments (TPE) susceptible to potential drought stress, with a focus on the widely adopted upland variety, Nerica 4 (N4). The study utilizes simulations spanning from 2012 to 2022 to describe the dynamics of yield patterns in the region.

Mechanistic crop modeling functions as an approximation of plant behavior in drought stress response, reacting to environmental data and crop parameters according to plant responses. The intensity and temporal evolution of drought stress form patterns through extensive simulations spanning ten years in the complete regions of Casamance. Through observation, mechanistic crop models are calibrated, with drought stress characterized by soil water availability and genotype response. Drought stress, in this context, relies on the water balance integrated into the mechanistic crop model. The model quantifies drought stress by computing a stress factor representing its intensity. This computation is performed daily, shaping the stress intensity profile, identifying its occurrence and trend over time.
The accuracy and confidence of these models depend on the quantity and quality of data available. In the Casamance region of Senegal, data mainly cover grain yield in kilograms per hectare, soil features from laboratory measurements, and meteorological data from local stations. However, insufficient data on yield performance, climate, and soil remains one of the primary limitations when simulating entire regions. In this context, the utilization of satellite data to feed mechanistic crop models, with the environment climate and soil, contributes to identifying drought stress patterns across complete regions. This research describes the drought stress patterns calculated using a mechanistic crop model fed by

environmental satellite data. It also emphasizes the differences in drought simulation compared to using data from meteorological stations and soil measurements.
The outcome of his research is the Target Population of Environments (TPE) for drought stress, which reflects clusters of drought stress patterns, capturing spatial and temporal variability to describe environments associated with each cluster. These environments are defined by their climate and soil attributes.

ChloroKB web application and The Arabidopsis Leaf Quantitative Atlas: tools for modelling plant metabolism

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ChloroKB is a regularly updated knowledge base (http://chlorokb.fr) designed for the metabolic reconstruction of the model plant Arabidopsis. It brings together curated textual and quantitative information on proteins, unidentified genes, and metabolites, presenting them in interconnected maps that depict metabolism within cellular compartments using CellDesigner semantics. This tool aims to bridge the divide between human-understandable biochemical representations and computer-based modelling. The uniqueness of ChloroKB lies in its synoptic views of complex biochemical processes, with contextual representation of protein actors not only in chemical reactions but also in sophisticated complexes, transport steps, and short-term regulatory mechanisms.

Recently, we developed a quantitative atlas of a virtual Arabidopsis leaf (n°6), compiling data scattered throughout the literature. This atlas provides quantitative information (volumes, numbers) about 15 cell types and their organelles for a reference leaf at a precise developmental stage and under specific growth conditions. Integrated data in a calculation table allow the derivation of additional metrics. Both ChloroKB and the Quantitative Atlas of Arabidopsis Leaf n°6 are tools dedicated to modelling plant metabolism. I'm keen to discuss how these tools could be enhanced to further support the modelling of plant metabolism.

[1]Tolleter D., Smith EN, Dupont-Thibert C., Uwizeye C., Vile D, Gloaguen P., Falconet D., Finazzi G., Vandenbrouck Y., and Curien G. (2024) The Arabidopsis Leaf Quantitative Atlas: a cellular and subcellular mapping through unified data integration. Quantitative Plant Biology (https://dx.doi.org/10.1017/qpb.2024.1)

Modeling plant water uptake : from cross sections to root architecture

Marco D'Agostino[1], Rémy Schoppach, Adrien Heymans[2], Valentin Couvreur[1], Guillaume Lobet[1,3]

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The efficiency of water uptake by plants is closely tied to their root system architectures and the anatomical features of individual root segments. Local root anatomies strongly influence the capacity of a root segment to transport water from the soil into the xylem vessels (radial conductivity), and along the xylem vessels network (axial conductance). Structural factors that influence local radial and axial root hydraulic properties have been extensively studied in monocots, especially maize, but not for dicots, where important anatomical differences could represent significant consequences in hydraulic dynamics. Namely, monocot and dicot root can differ in terms of developmental anatomy, the presence of secondary growth in woody dicots, and types and timings of apoplastic barriers. These differences highlight the need to improve our knowledge on how secondary growth combined to specific deposition levels and developmental anatomy define and influence radial and axial hydraulic properties at the cross-section scale.

In this work, we update and use structural and functional models to study the influence of anatomy (including secondary growth), hydrophobic depositions levels (suberin and/or lignin in endo- and/or exodermis) and subcellular hydraulic properties (aquaporins contribution) on local root hydraulic properties. We also investigate the consequences of such properties on root system hydraulic architectures. We use tomato (Solanum lycoperiscum L., var. Moneymaker) as a model of secondary growth dicotyledon.

We explicitly show that:

1. Exodermal apoplatic barriers (lignin cap and suberization) are powerfull at reducing radial conductivity, but in a lesser extent than endodermal barriers.
2. The influence of aquaporin contribution on radial conductivity is reduced in suberized parts of roots, as shown in previous litterature.
3. Secondary growth compensates the effect of hydrophobic barriers and prevents the radial conductance to collapse, allowing for highly suberized roots to still contribute to radial water uptake.
4. Secondary growth and dicot developmental anatomy are required to increase and maintain high axial conductance, to sustain water uptake along the whole soil profile.

Multiscale integrative modelling of plant growth

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The plant cell wall, a complex network of polymers and proteins, constitutes a fundamental element of plant cell architecture, exhibiting remarkable properties. A pivotal enigma revolves around the mechanism enabling this wall to expand while enduring the stress induced by turgor pressure. Around 100 years of experiments has led to propose different molecular mechanisms underlying growth and morphogenesis processes. Currently, the "Biomechanical Hotspot" model is the most accepted, coexisting with other emerging models such as "Expanding Beam" or "Ca-Pectate Exchange" models. These three models are non-mutually exclusive. To deepen our understanding on how they could work in parallel, we adopt a modelling approach aimed at integrating various hypotheses to simulate and potentially predict cell wall expansion. In this poster, I will present advancements in a numerical model for growth and morphogenesis based on cell wall mechanical and biochemical characteristics utilizing nonlinear 3D finite element analysis. It is implemented to have explicit dependency of variables to experimental data. To investigate separately tip-growth to tissue diffuse one, we explore respectively root hair and pavement cell expansion. In addition, we will integrate biochemical processes, such as rapid regulatory mechanisms, into a dynamic hybrid model. Through this integrated model, we hope to gain valuable insights into the cell wall expansion behaviour.

Learning plant cell division rules using deep neural networks

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Plant embryo development is an intricate process whereby a complex organism arises from a single cell. At the cellular scale, this process hinges on the fundamental mechanisms of cell division and growth. Cell division, in particular, plays a pivotal role by reshaping tissue properties like mechanical constraints and topology, thereby influencing morphology. Predicting the positioning of a new cell wall during division is thus crucial for understanding morphogenesis. Early attempts to predict cell division positioning relied on geometric approaches based on the shape of the mother cell. While geometry contributes to division plane positioning, other factors like chemical signaling, mechanical constraints, and tissue-scale optimizations also exert influence. However, deciphering how each factor impacts division remains challenging. Current models, whether based on geometry, stresses, or other properties, are typically rule-based, incorporating manually defined rules that may contain human biases or overlook certain aspects. It is then difficult to define whether the data does not fit any rule or if the right rule was simply not identified. In *A. thaliana* embryos, a geometric division rule successfully fit the observed divisions from stage 1C to stage 32C, with the exception of the stage 16C basal intern cells (Moukhtar et al. 2019, Laruelle et al. 2022). Do these latter cells follow a different rule from the previous stages, or is there an alternative common rule? To ensure that the proposed division rule aligns as closely as possible with observations, we propose a method to automatically learn predicting cell division plane positioning in a supervised framework. Leveraging U-Net3D, a deep learning architecture tailored for biological image segmentation, we train a model to approximate division rules based on an image dataset of before/after division pairs. This formulation transforms the prediction of division plane positioning into a more accessible segmentation task. Additionally, representing mother cells by their 3D image masks enables the model to approximate a strict geometric division rule from fully preserved geometric information. We conducted multiple experiments to assess the potential and limitations of this novel approach. We first evaluated the network's ability to learn a simple division rule using synthetic shapes like cuboids and ellipsoids. Subsequently, we tested the model's generalization capability across different shapes and its performance in approximating complex division rules. Finally, we applied the approach to real *A. thaliana* embryo cells spanning developmental stages 1C to 32C. We trained the model to learn stage-specific division rules and subsequently a universal rule applicable across all stages.

Geometric and mechanical guidance: role of stigmatic epidermis in early pollen tube pathfinding in Arabidopsis

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A major question in plant reproduction is how pollen tubes sense and interpret female cues to navigate in the pistil and maintain the directionality towards their goals. Throughout its journey, the pollen tube advancement depends on a cooperative cell-to-cell communication network starting when the pollen grain makes the first contact with the stigmatic papillae, located at the pistil's receptive tip. As the pollen tube emerges from the grain, it invades the papilla cell wall and progresses engulfed within this rigid layer towards the stigma basis. Thus, the behaviour of the pollen tube is intricately linked to the biological and physical properties of the invaded papilla cell and despite its importance, this initial phase of the pollen tube journey remains elusive. Here, we developed a multidisciplinary approach combining methods and concepts from biology, geometry and mechanics to dissect this original growth process. We used computational modelling to explore the effects of a wide range of papilla geometries on tube paths while maintaining constant cell wall properties, and estimated the magnitude of the elastic energy required for a tube to grow confined within two elastic layers. By comparing the model predictions to experimental data, we propose a mechanism wherein the guidance of the pollen tube is driven by the quasi-cylindrical geometry of the papilla and the elasticity of its cell wall.

Numerical reconstruction of plants seeds for morphogenesis analysis

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Arabidopsis thaliana seeds are organs of choice in the study of morphogenesis and its regulation. During development, seed growth is promoted by the pressure generated in the endosperm under compression and restricted by the mechanosensitive stiffening of the walls in the surrounding seed coat (*Creff, A. & Ali, O. et al. 2023*). While this mechanosensitive regulation, formalized by an incoherent feedforward loop, account for final seed size and shape emergence; experimental data suggest that it could be controlled by inner layers of the seed coat. To assess the role of inner tissue organization on seed development, we built relevant data structures that allow fine analysis at the cellular level of the entire seed coat.

We developed a numerical study driven by an image analysis pipeline combining high resolution microscopy and computational methods to extract meshes compatible with mechanical simulations. We reconstructed numerically the full 3D multilayered structure of Arabidopsis seeds encompassing tissue topology and unraveling geometrical properties at the cellular scale.

References

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Resource allocation modeling for autonomous prediction of plant cell phenotypes in constrained growth conditions

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Predicting the plant cell response in complex environmental conditions is a challenge in plant biology. We developed a resource allocation model of cellular and molecular scale for the leaf photosynthetic cell of *Arabidopsis thaliana*, based on the Resource Balance Analysis (RBA) constraint-based modeling framework. The RBA model contains the metabolic network and the major macromolecular processes involved in the plant cell growth and survival and localized in cellular compartments. We simulated the model for varying environmental conditions of temperature, irradiance, partial pressure of CO2 and O2, and compared RBA predictions to known resource distributions and quantitative phenotypic traits such as the relative growth rate, the C:N ratio, and finally to the empirical characteristics of CO2 fixation given by the well-established Farquhar model. In comparison to other standard constraint-based modeling methods like Flux Balance Analysis, the RBA model makes accurate quantitative predictions without the need for empirical constraints. The RBA model is currently under calibration on dedicated datasets composed of non-limiting (control) as well as limiting growth conditions (water -W- and nitrogen -N- limitations), and will be finally challenged to predict a range of combined stress (W*N) conditions and for two Arabidopsis accessions. Altogether, we show that RBA significantly improves the autonomous prediction of plant cell phenotypes in complex environmental conditions, and provides mechanistic links between the genotype and the phenotype of the plant cell.

Network Analysis for Plant Extracellular Signals

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Constant efforts are directed towards further developing non-invasive measurement systems to interpret and explore physical and biological responses of plants with respect to their surroundings. A class of sensors that has gained popularity are wearable sensor systems because they show promising results in better translating unique responses to environmental cues in real-time. Our focus is guided towards wearable sensors that measure plant extracellular electrical signals at multiple locations on a growing plant. Our work presents an open-source sensor which has the ability of measuring at 8 different locations of a plant. For the scope of our study, we track the extracellular signals at 5 locations at a frequency of 5Hz. Probes are placed along individual pea plant stems while subject to different lighting conditions. The data is collected bi-directionally enabling the network analysis of signals flowing in both directions: top-bottom and bottom-top. A network analysis enables a different perspective on how the electrical signals are propagated throughout a plant body through the coordination of cellular and physiological processes, and how similarities between signals are changing over time. We select the stimuli of light as it is one of the most critical environmental factors influencing plant growth, development, and behavior. The presence, absence and duration of light exposure are key factors that plants use to maintain their circadian rhythms. We present our case study which collects data over the period of 72 hours on pea plants that were subject to continuous light or full darkness. Their results are compared to a control group with a lighting schedule of 16 hours of light and 8 hours of dark. Signals are interpreted through a network formulation where the nodes are the locations along the plant stem and the edges are built based on similarity scores between signals that are computed via dynamic time warping. The dataset collected was collapsed in different time chunks, starting with a granular approach investigating the representation of 72 hours, 24 hours periods, 8 hours periods and followed by a temporal graph analysis with a sliding window to understand how edges evolve overtime. We provide a methodology for collecting such data as well as an open-source sensor to enable the community to have access to this technology. We explore degree centrality to express which locations along the stem are of importance during lighting schedules as well as graph density to interpret if the plant is under stress or not.

Metal nanoparticles pass through protoplast interfaces and intracellular distributions

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Abstract

Heavy metals absorbed and accumulated by plants from the soil can pose a health risk if they enter the food chain through crop uptake, which is a complex biological process that depends on multiple factors. To understand how the size and surface properties of metal nanoparticles affect the uptake and intracellular accumulation in plants, we prepared fluorescent PEG-coated gold nanoparticles of different sizes (5-50 nm) and surface functionalities: positive, negative and neutral charge. We quantitatively investigated nanoparticle uptake and accumulation in Arabidopsis Thaliana protoplasts using confocal fluorescence microscopy. The results show that the number of particles absorbed is inversely proportional to the size of the nanoparticles. Furthermore, positively charged nanoparticles rapidly accumulate on the surface of the protoplasts whereas negatively charged particles accumulate more slowly on the cell surface and neutral nanoparticles rapidly penetrate into the protoplasts. All charged nanoparticles are found to accumulate in the cytoplasm and cellular organelles such as lipid droplets and vacuoles. These findings indicate that the uptake and intracellular accumulation of gold nanoparticles in Arabidopsis protoplasts are significantly affected by their surface charge and size and give a better understanding of metal nanoparticle uptake and accumulation in plants.

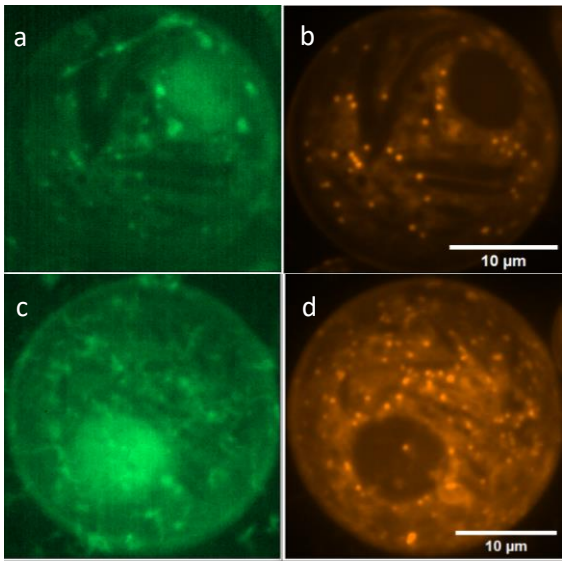

Figure 1. Distribution of green fluorescent gold nanoparticles after a) 2 hours and c) 4 hours culture in protoplast. Liposome structures in protoplasts fluoresce orange by Nile Red staining.

4D Characterization of Plant Cell Wall Enzymatic Hydrolysis in Highly Deconstructed Samples

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Transforming plant cell walls into bioproducts represents a crucial move in shifting away from reliance on fossil carbon to renewable energy and material sources. The challenge in the transformation of the cell wall lies in addressing its intrinsic resistance, known as recalcitrance, to enzymatic deconstruction. Over the past decades, research efforts have largely focused on identifying markers of recalcitrance at the nanoscale. Consequently, the enzymatic deconstruction of plant cell walls at cell and tissue scales remains comparatively underexplored. To fill this gap, we developed a protocol to acquire time-lapse images of spruce tree samples during enzymatic hydrolysis involving sample preparation, pretreatment and confocal imaging generating highly deconstructed datasets. The primary challenge lay then in analyzing the datasets exhibiting a high degree of deconstruction. We therefore developed a computational pipeline specifically devised to handle samples undergoing significant deconstruction and deformations. The pipeline involved an adapted spatial information propagation strategy to first segment the image before hydrolysis which could possibly exhibit a tilt by imposing constraints on the watershed algorithm. To segment the images during hydrolysis, the pipeline included a propagation strategy adapted for highly deconstructed samples where the sequence of images was divided into sequential clusters ensuring that the final image of a cluster is also the first image of the subsequent cluster. Transformations are then computed within each cluster by registering the starting image of the cluster with the subsequent images within that cluster. Starting from the first cluster including the image before hydrolysis, these temporarily constrained transformations are then applied to the segmentation of the initial image of the cluster yielding the segmentations of the subsequent images in the cluster. By limiting the registration algorithm to individual clusters, this approach allows segmentation and tracking of images of highly deconstructed samples. Using this approach, we also computed dynamics of cell wall autofluorescence intensity values which is then used to develop mathematical models of cell wall deconstruction assuming that the evolution of the autofluorescence values is a proxy for enzymatic deconstruction. Overall, the results shed light on the underlying parameters of the cell wall deconstruction with quantitative relationships across scales.

Morphometry and growth of wheat grain by registration of 3D tomography image

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Wheat grain is one of the most important staple foods in France and in the world. A better understanding of its growth is necessary to maintain sufficient production in a context of global climate change. We used X-ray micro-tomography on grains at different stages of development to quantify changes in morphology of wheat grain according to its development, and to identify regions of strong growth.

X-ray micro-tomography produces 3D images of the grains, which make it possible to study the external morphology of the grains but also to explore their internal structure in a non-destructive way. Images of satisfactory contrast and resolution were obtained even for young and highly hydrated grains. We developed a 3D image processing workflow to quantify grain growth. A segmentation step allowed identifying the grains, as well as the internal and external regions. The global 3D morphology was quantified using several morphometric features: grain dimensions along the main axes, and volume of the different compartments. The evolution of the features makes it possible to describe the overall growth of the grain.

To better identify growth patterns along the grain, we have implemented a shape registration approach. The 3D images were converted to triangular meshes, and a group-wise registration algorithm produced a grain shape representative of each stage. We then computed the geometric transformations, in the form of deformation fields, which depict the deformation of the grain between successive stages. The spatialized analysis of the deformation fields then makes it possible to identify regions presenting differentiated growth patterns. In particular, the upper part of the grain presents significant growth.

This work opens many perspectives for the understanding of mechanisms involved in wheat grain growth, in particular to validate or feed morphogenesis models. The approach is generic and can be adapted to other types of seeds observed by 3D imaging, or even to other types of plant organs.

Control of the spiral phyllotaxis from a single stem cell in the moss *Physcomitrium patens*

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*(*denotes equal contribution)*

The architectural plan of an organism determines its main axes of symmetry and is key to position each organ relative to each other with precision and robustness. In plants, botanical elements such as leaves are arranged following a periodic and geometric pattern called “phyllotaxis”, which can be spiral, whorled or opposite. This pattern emerges at the cellular level from the shoot tips where stem cells are located. So far, phyllotaxis has mainly been studied in flowering plants with shoot tips composed of hundreds of cells. Unlike flowering plants, the shoot tip of the model moss *Physcomitrium patens* is composed of a single stem cell, known as the apical cell. As a result, the position of each new leaf strongly depends on the division pattern of the apical cell. However, the mechanisms that control the positioning of the apical cell division plane to pattern moss phyllotaxis remain to be discovered.

Within this framework, my project aims to decipher the molecular and biophysical mechanisms that control spiral phyllotaxis in *P. patens*. Using a combination of quantitative time-lapse imaging, cellular shape analysis and modeling in various transgenic lines, I have been able to provide a quantitative description of the division dynamics at the moss shoot apex with a cellular resolution. These results bring the first insights into how a single stem cell directs its division plan to generate a complex and robust biological pattern.

Integrated Proteomics and Metabolomics Emphasized Nutritional Benefits Driven by Lentil (*Lens culinaris* Medik.) Seed Germination.

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Lentil (*Lens culinaris* Medik.) is an annual legume rich in protein, fiber, vitamins, and minerals. Germination is a crucial process in the lentil life cycle with potential implications for both agronomy and food processing. However, knowledge about lentil seed germination has been limited. Our study aims to address this gap using a systems biology approach. We investigated lentil seeds at different germination stages (dry seed, 12h imbibition, and 24h imbibition) and two temperature conditions (25℃ and 30℃) using physiological germination counting and Multi-Omics Integration (MOI) approaches, including metabolomics and proteomics. We identified differential accumulation of 88 out of 300 metabolites and 136 out of 1275 proteins under different germination/temperature conditions. Due to the lack of complete lentil genomics annotations, we further improved the automatic functional annotation of lentil protein-coding sequences based on homologous alignment against well-annotated plant genomes. Through the integration of Multi-Omics signatures, metabolite/genomic annotations, and pathway analysis, we identified metabolic pathways and biological processes related to protein metabolism, RedOx metabolism, and anti-nutritional compounds. This descriptive analysis using a Multi-Omics approach provides valuable insights into lentil seed germination for the first time. The metabolic dynamics observed in this study can serve as a guide for improving the nutritional quality of germinating lentil seeds as food. Lentil germination has potential implications for food processing and nutrition, and our findings contribute to a better understanding of the underlying molecular processes involved in lentil seed germination.

Modeling ovule curvature

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Tissue morphogenesis remains poorly understood. In plants, a central problem is the interplay between the individual growth of mechanically connected cells and tissue-level processes that lead to emergent morphologies and properties. We use ovule curvature as a model to address this aspect, taking a comparative approach that exploits the diversity of ovule curvature across angiosperms. We apply advanced imaging and machine learning based cell segmentation to generate 3D digital ovules with single cell resolution. This allows us to investigate the hidden functional complexity of the 3D cellular architecture underlying ovule curvature. We then combine quantitative comparative morphometry to explore similarities and differences in the 3D cellular architectures of ovules from a variety of angiosperm species. The cellular parameters obtained are used in finite element modeling (FEM) to develop plausible models that explain the differences in ovule curvature, which in turn are functionally tested by genetic perturbations where possible. Here we present the results of our work on two species with differently shaped ovules: *Arabidopsis thaliana* and *Cardamine hirsuta*. We first generated 3D digital atlases of ovule development at single cell resolution for both species. We then focused on “kink formation”, a genetically distinct first step in ovule curvature development that is provoked by the growth pattern of the central region of the young ovule, the chalaza. Ovules of the two species differ in their degree of kink formation. We first inferred differential growth patterns from an analysis of the respective 3D cellular architectures of the chalaza. We then incorporated this information in 2D tissue-based FEM simulation representing a mid-sagittal section of the ovule. We further challenged our 2D finite element models by simulating the inferred growth patterns in the *ino-5* mutant of Arabidopsis which exhibits a polarity switch in kink formation. The results suggested that subtle differences in cellular growth patterns in the central region result in striking differences in kink formation. Our work demonstrates the power of combining comparative 3D cellular morphometry with FEM. It highlights the importance of internal tissues down to their cellular architecture, in inducing the morphogenetic properties of a growing organ.

Robustness in the morphogenesis of Arabidopsis sepals

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Robustness in organ development is the formation of the reproducible organ sizes and shapes despite perturbations in the environment, stochastic (or random) gene expression, and cellular variability. Development is remarkably robust, producing plant organs such as leaves and sepals with the same size and shape repeatedly from individual to individual. Yet, these reproducible organs are composed of cells that are highly variable in size, shape, growth, and division. My laboratory uses a computational morphodynamics approach, including genetics, live imaging, image processing, mechanical assays, and computational modeling, to elucidate the mechanisms that produce robust organ size and shape from cellular heterogeneity. We use *Arabidopsis* sepals as a model organ because there are four sepals on each flower; this enables statistical tests of robustness. To identify mechanisms generating robustness we have screened for *variable organ size and shape* (*vos*) mutants that disrupt the robustness of sepal morphology (Hong et al., 2016). These studies reveal mechanisms through which individual cells, which are often highly variable, collectively give rise to complex organs with reproducible and robust sizes and shapes.

The mechanism to make puzzle shaped cells is broadly conserved in higher plants

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Puzzle-shaped cells in the shoot epidermis are thought to alleviate mechanical stress during multidirectional growth in many plant species. Yet, the absence of such cells in numerous plants has sparked debate over this theory. Our extensive analysis of both current and fossilized plant species reveals that the ability to develop puzzle cells is a common but variable trait. This variability is influenced by factors such as the type of organ, the stage of development, and environmental conditions, often concealing the presence of the trait. Through computational models of *Arabidopsis thaliana* and maize (*Zea mays*), we discovered that lobe formation is a dynamic process, closely tied to a plant's growth history and environmental context. Additionally, we found that the suppression of the ability to form lobes, whether due to genetic mutations or pharmacological interventions, significantly impacts plant development, requiring alternative growth adaptations. Our findings suggest that the formation of puzzle-shaped cells likely represents a broadly conserved response among higher plants to a mechanical developmental constraint triggered by growth and mechanical stress.

Towards an integrative view of plant cell division in a time-resolved canvas describing and quantifying the dynamics of subcellular structures during the cell cycle in higher plants

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The remarkable robustness of multicellular development and morphogenesis in eukaryotic organisms emerges from multiscale interactions between cell-autonomous activities, local cell-cell interactions and long-distance signaling and cross-talks at the organ and organism levels. Plant multicellular development heavily relies on a precise spatio-temporal control and coordination of division and growth. This coordination is brought about by a complex interplay between the nucleus, the cell-cycle machinery and other cellular structures, among which the cytoskeleton and the plasma membrane play cardinal roles.

Several pieces are missing to the puzzle, and many questions are pending, related to the molecular/cellular processes and networks involved, their sequence and link to the cell cycle, the nature and timing of initial cues driving cell division plane positioning,

We are in the process of building an integrative view of plant cell division is a time-resolved canvas describing and quantifying the dynamics of subcellular structures during the cell cycle. The framework will be amended and completed in the future on an open/community basis.

Finding the determinants of various 3D growth strategies in brown algae

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Three-dimensional (3D) growth is considered an intricate morphogenetic process, and in brown algae, as in plants, it relies on the specific location of the cell division plane. Interestingly, cell division occurs differently in brown algae than in plants. Indeed, the cellular components involved in determining the position of the division plane are also different. Therefore, the rules determining the orientation of division planes during mitosis in brown algae appear to be different from those of land plants but are still to be unraveled.

Our laboratory is investigating the 3D growth strategies of three brown algae species: *Sphacelaria rigidula*, *Fucus serratus* and *Saccharina latissima*, each employing a distinct 3D growth strategy. *Sphacelaria* uses a strategy whereby the apical cell grows along a single axis and then sub-apical cells divide to grow in other dimensions. In contrast, *Fucus* initiates cell division without cell expansion, a process reminiscent of early embryo segmentation in metazoans.

In these algae, we aim to discover the cellular and mechanical actors that determine when, where and in which orientation the cells involved in 3D growth divide. To obtain a holistic view of these developmental processes, I am adapting *in vivo* time-lapse microscopy and *ad-hoc* image analysis to these organisms. This will provide us with quantitative and qualitative data to build a comprehensive and dynamic map of the position and orientation of the cell division planes during algae's 3D growth.

Modelling potato primary and secondary metabolism captures the principles of plant growth and defence under biotic stress

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Solanum tuberosum is among the most important food crops and a model tuber crop species. It is also of interest to establish this crop as a model system for studying growth-defence (G-D) trade-offs. Plants enter a defensive state in response to environmental stresses or pathogens, rerouting many resources from their primary growth objective and thus performing well below their maximum potential. Understanding such tradeoffs can help us develop improved crop varieties with increased stress tolerance, improving yields and quality.

To investigate G-D trade-offs in the context of metabolism, we developed a compartmentalised genome-scale metabolic model of potato metabolism (PotatoGEM). It contains information on the stoichiometry of thousands of biochemical reactions, connecting them to the genes encoding the enzymes that catalyse them. We also curated and expanded the PotatoGEM secondary metabolism, capturing the full extent of it according to the MetaCyc database. The potato leaf biomass was quantified using in-house and published experimental data.

We employed the model to explore G-D trade-offs using our library of transcriptomics data, which included biotic stress responses to pathogens (Potato virus Y) and pests (Colorado potato beetle). This enabled the comparison of micro- and macro-biotic stress response mechanisms, and revealed the general principles of stress induced G-D trade-offs. Our results demonstrate how the curated model can be used to investigate multi-reaction trade-offs across primary and secondary metabolism, providing the basis for a metabolic perspective on G-D trade-offs typical across many plant species.

SKM and Booldog - From knowledge graph to dynamic Boolean modelling

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Abstract

The escalating challenges to global food security, driven by a burgeoning human population and the impact of climate change on agriculture, necessitate a sophisticated understanding of plant responses to stressors. Addressing this, our project harnesses systems biology to integrate and analyze the fragmented knowledge of molecular processes within plant cells. We introduce the Stress Knowledge Map (SKM), a comprehensive, openly accessible database constructed on a neo4j platform that includes genes, gene products, complexes, and metabolites through their molecular interactions. This integration facilitates not only the interactive exploration of complex biological networks but also serves as a foundation for advanced modelling techniques.

Given the limitations in capturing detailed kinetics for every interaction in SKM, we employ Boolean networks as a pragmatic approach to model plant stress responses. This methodology circumvents the need for exhaustive mechanistic details by simplifying the system into binary states ("active" or "inactive") for each node, derived from regulatory influences. Recognizing the inherent limitations of binary states to fully capture the nuances of biological systems, we extend our approach by translating Boolean functions into qualitative ordinary differential equations (ODEs) using various transform functions.

To support this systems biology framework, we developed BoolDog, a versatile Python package that enables the reading of regulatory and Boolean networks, execution of Boolean simulations and steady state analyses, and transformation of Boolean networks into continuous ODEs for continuous simulations. BoolDog is designed for interoperability and ease of extension, promoting its application in diverse systems biology research contexts.

Through these methodologies, our project advances the understanding of plant stress responses, provided powerful tools for the exploration, analysis, and modeling of complex biological systems that can be utilized in other biotechnological and biomedical fields.


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