Multiscale plant modelling and phenotyping in OpenAlea

Simposio Omicas 2022

16-18 Noviembre

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UMR AGAP Institute / Phenomen & Zenith, France

cirad

ÓMICAS

Inria
INVENTEURS DU MONDE NUMÉRIQUE

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agAP INSTITUT
Amélioration génétique et adaptation des plantes méditerranéennes et tropicales

PhenoMen Team

AGAP Institute (Genetic Improvement and plant adaptation)

Montpellier, France

Phenotyping and Modeling of Plants in their Agro-climatic ENvironment

(PhenoMEn)


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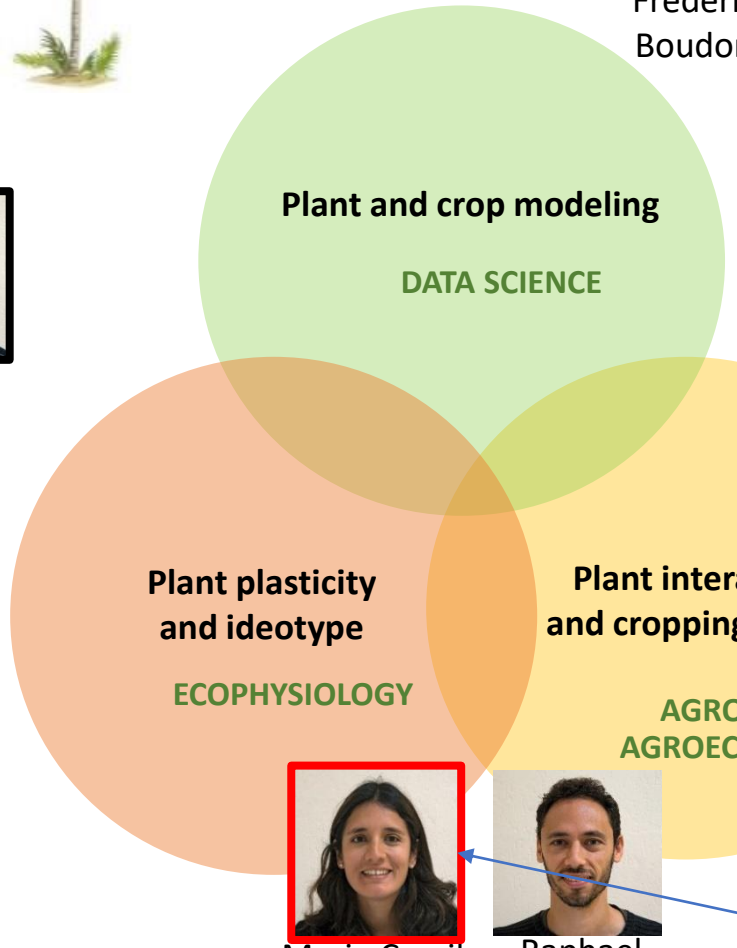


Myriam Adam


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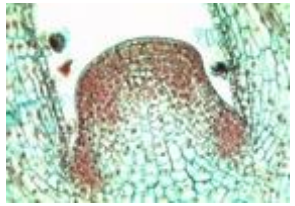
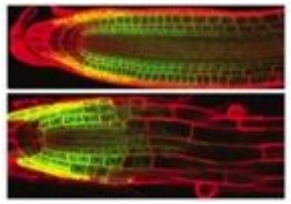
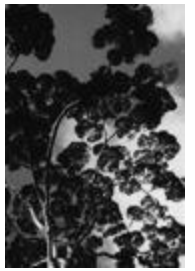
CIAT / Bioversity

Multiscale Plant Modelling

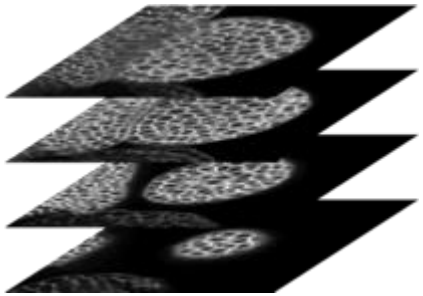
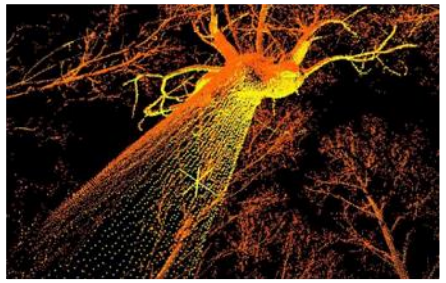
Different scales

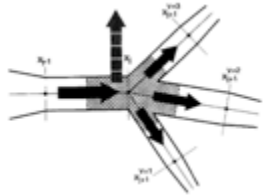




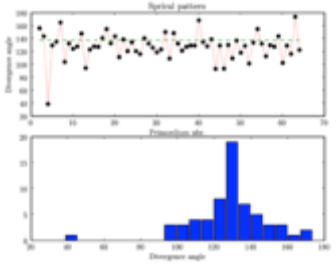

Data acquisition

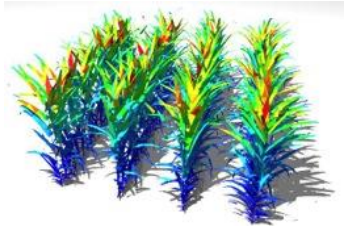
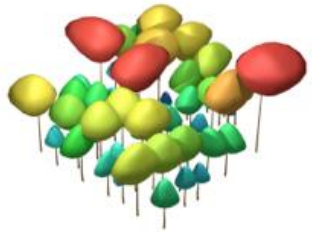

Modeling



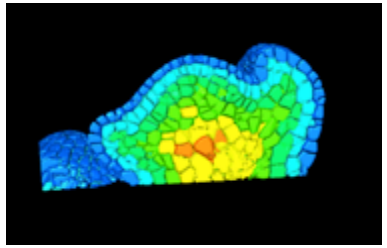
$$\frac{\partial}{\partial x}\left[K(x,P)\frac{\partial \Psi}{\partial x}\right] = c(x,P)\frac{\partial \Psi}{\partial t} + E(t)l(x)$$

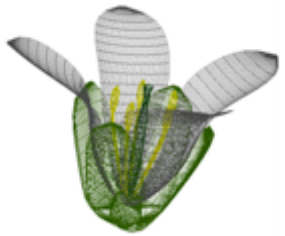



Simulation

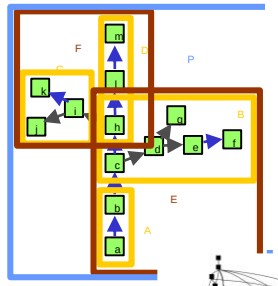



A diversity of modeling formalisms



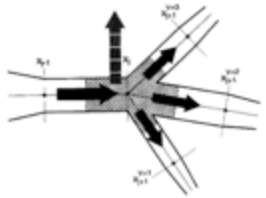


Geometrical models



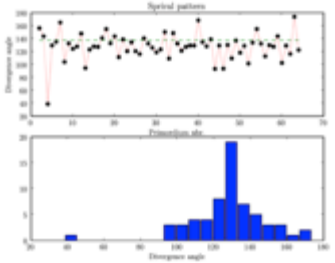
Fractals

Transport networks

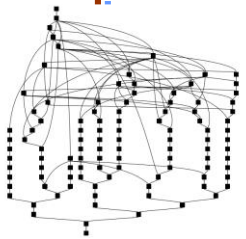


$$\frac{\partial}{\partial x}\left[K(x,P)\frac{\partial \Psi}{\partial x}\right] = c(x,P)\frac{\partial \Psi}{\partial t} + E(t)l(x)$$

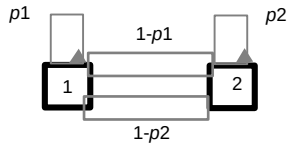
ODEs and PDEs



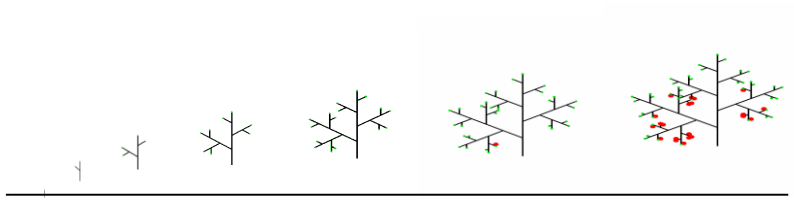
Statistical models



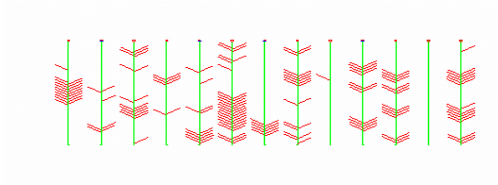
Graphs



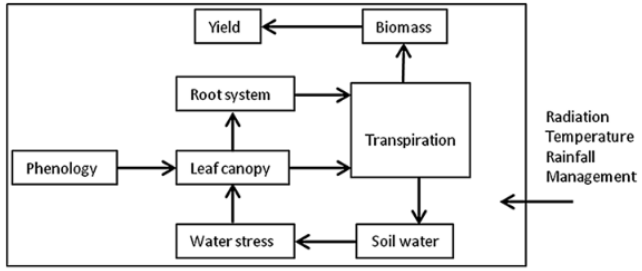

```
A(age) :age < T  --> I(age)[A(age+1)]A(age)
A(age) :age == T --> F
```



Dynamical systems with dynamical structure (e.g. L-systems, Growth Grammar)

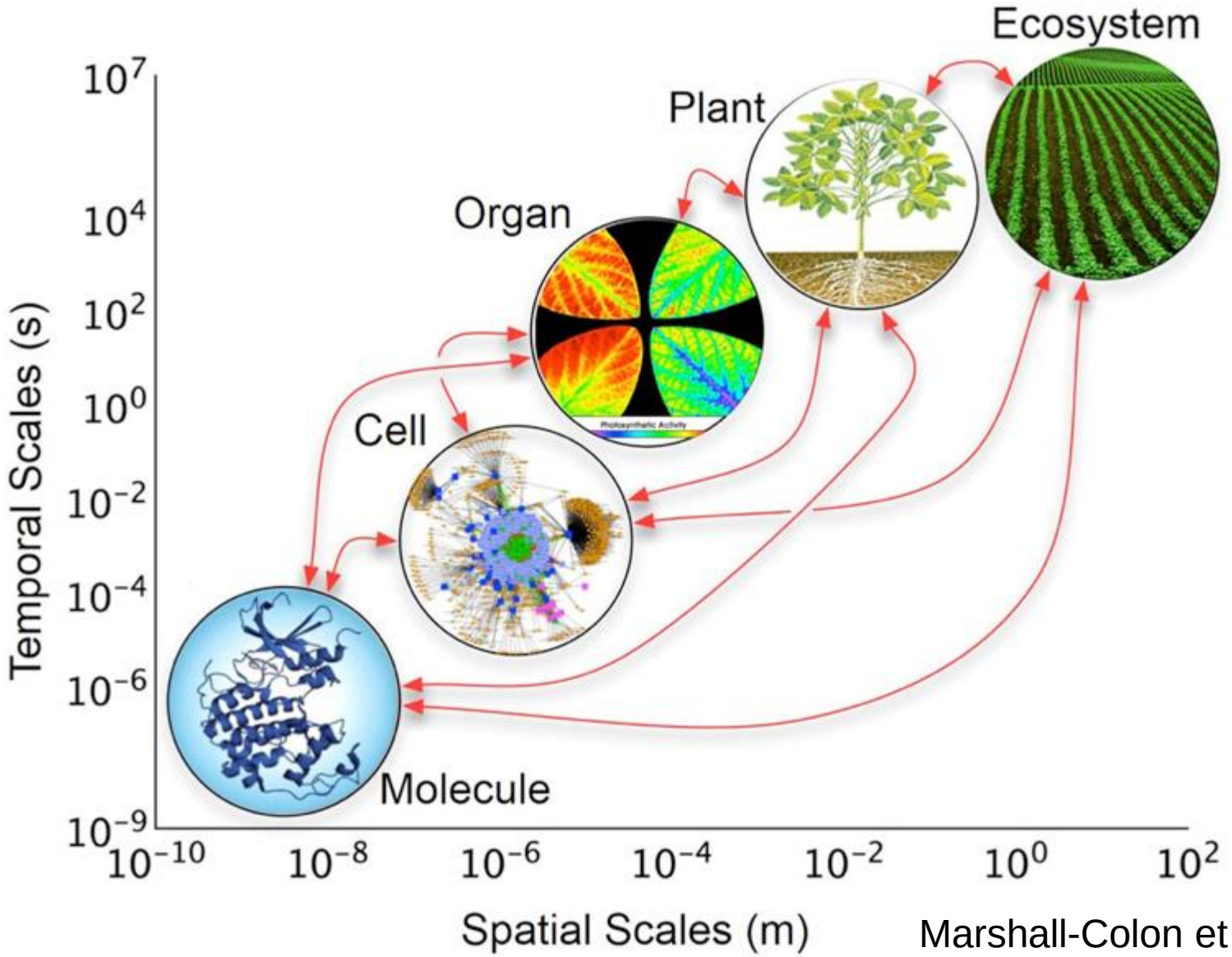


Stochastic processes



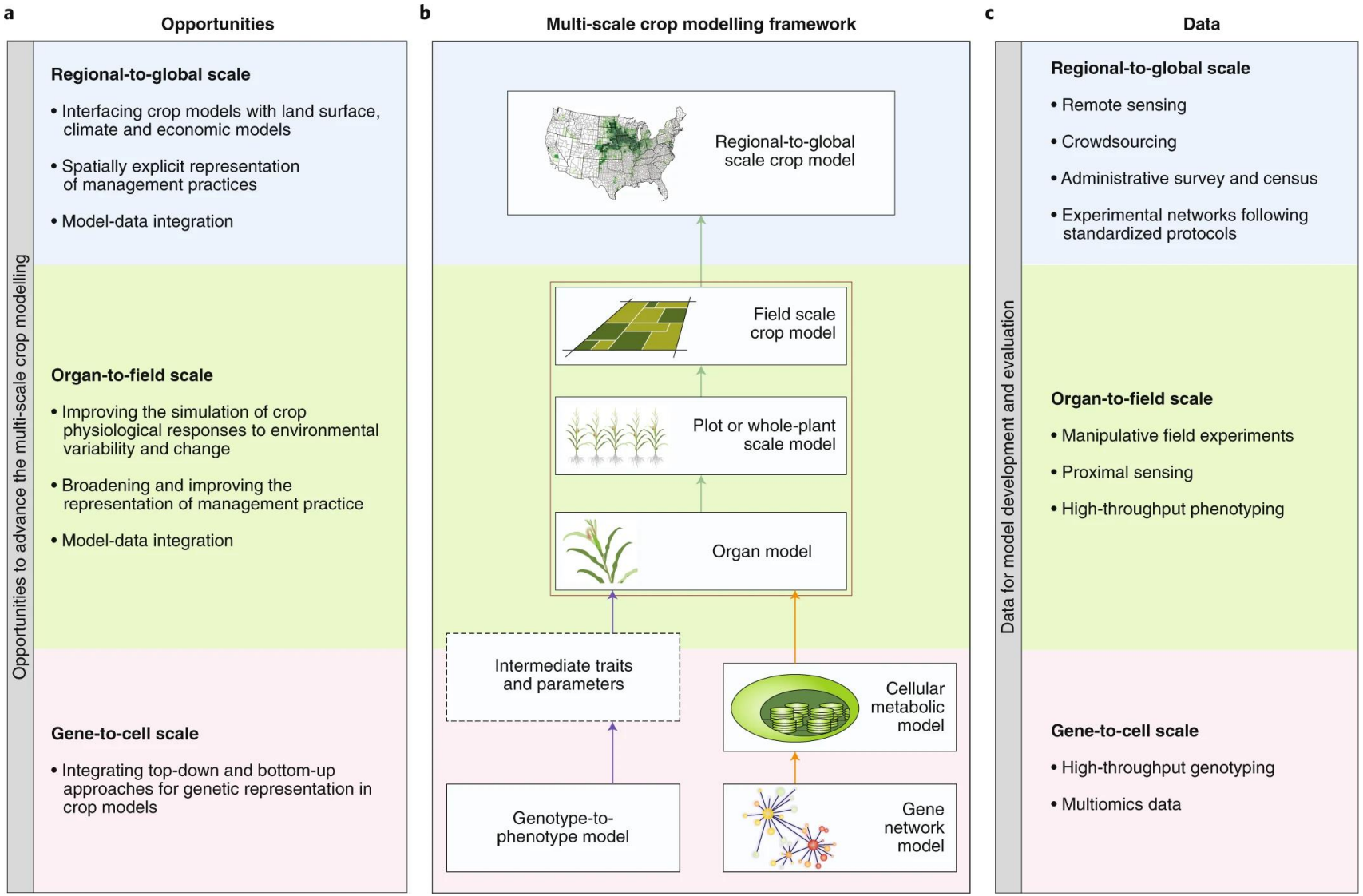
Process-based crop models

Complexity & retro-actions between scales



Marshall-Colon et al., 2017

Multiscale crop & plant models



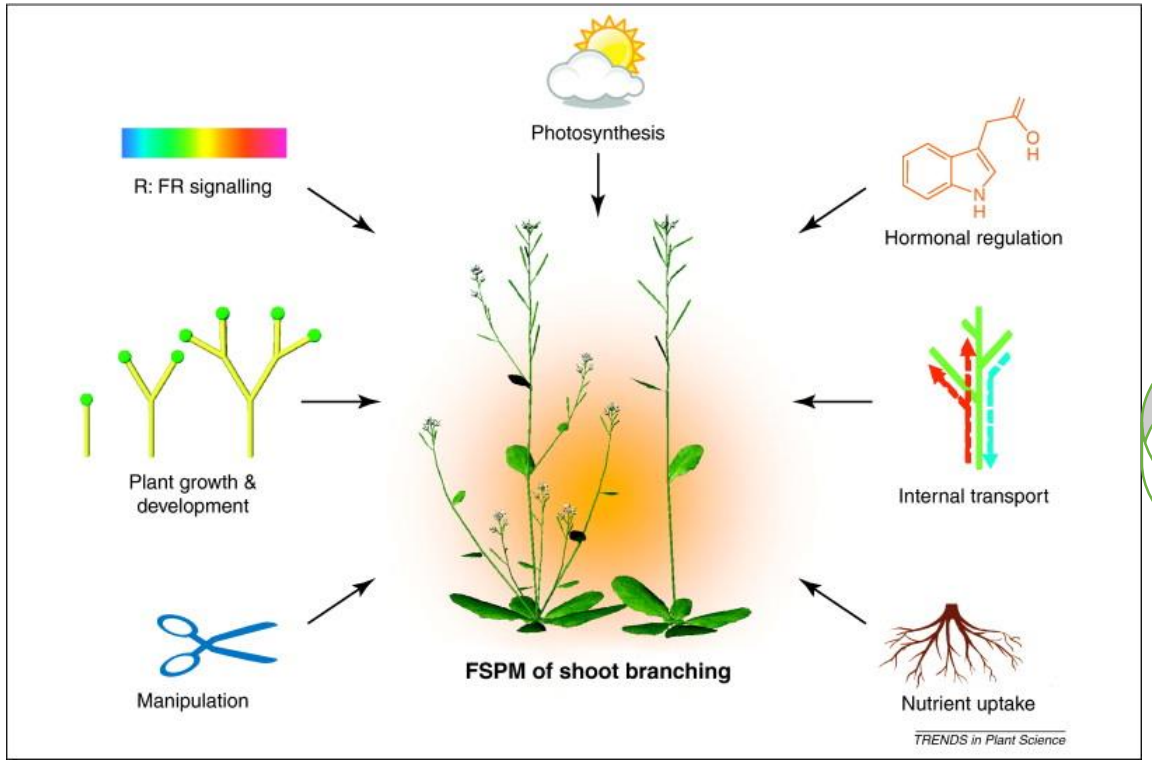
Crop Model (PBM)

Plant Model (FSPM)

Peng et al., 2020, Nature Plants

Functional-Structural Plant Models (FSPMs)

Functions

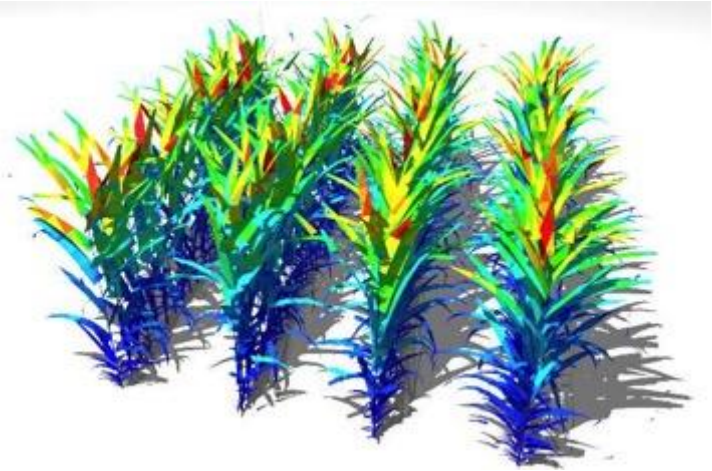


Evers et al., 2011, TIPS

3D plant structure

GreenLab, de Reffye et al, 2020, Ann. Bot.

Roles of Plant Structure (FSPM)

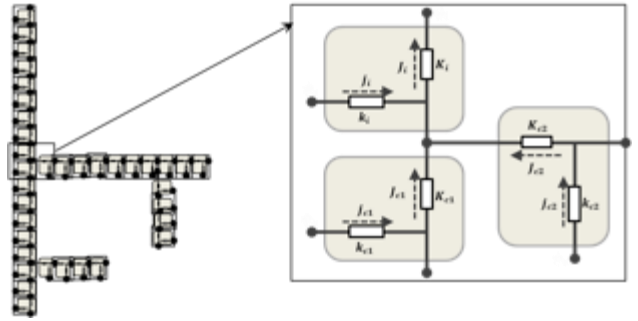


Plant structure as an interface

- Plant / environment interactions mainly depend on plant geometry (e.g. light interception)

Plant as a network

- Plant structure provides the support of fluxes (water, sugars) and signals (hormones, meca)



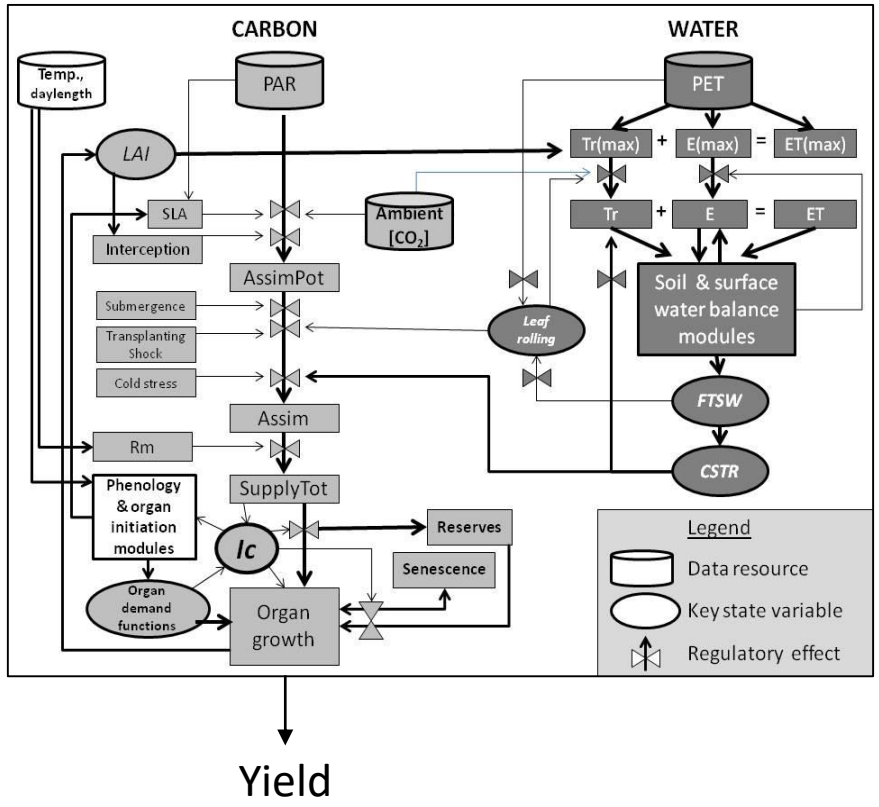
Plant as a developing organism

- Functional structural plant models (FSPM)

Godin & Sinoquet, 2005, New Phytol.

Why and how crop modeling and physiology can help?

- Knowledge on biological processes & their response to the environment
- Dynamics of yield elaboration (biomass, grain..)
- Interactions, trade-offs among processes difficult to look at experimentally
- Genotype X Environment X Management (GxExM)
- Yield & intermediates variables (stress indices: water, N…)
- Soil / Crop / Atmosphere



High-Throughput Phenotyping (HTP)

F. Tardieu, L. Cabrera-Bosquet, T. Pridmore T, M. Bennett (2017) Plant Phenomics, From Sensors to Knowledge. Current Biology 27(15):R770-R783

- Study the impact of different environmental conditions for various genotypes
- Quantify plants by Imaging
- Automatic High-throughput system
  - Imaging (12 sides & top view)
    - 250 GB/day
    - 10 TB/essay
    - 30 TB / year
  - Watering and whole-plant transpiration
    - Temperature + weight measured every day

Scientific Challenges

- Various **models** at different scales (FSPM & Crop models)
- Very fast **improvements** of Phenotyping (sensors, methods)

However,

-> How to **integrate** various multi-disciplinary models into a same **platform?**

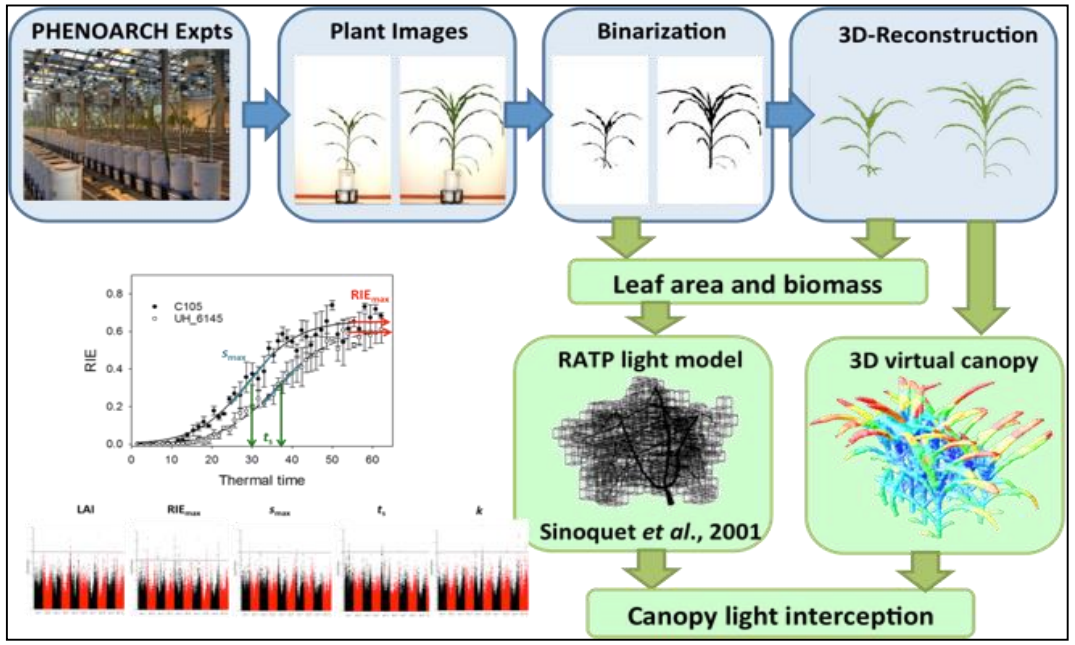
-> How to **automate phenotyping** of 3D architecture and development at high-throughput on large panels?

-> How to **connect phenotyping & modelling** (in-silico experiments)**?**

-> How to **enhance model reuse** between modelling platforms**?**

Outline

- **OpenAlea Software Platform**
- HTP Shoot Phenotyping & Modelling
- HTP Root Architecture & Modelling
- Crop modelling framework interoperability

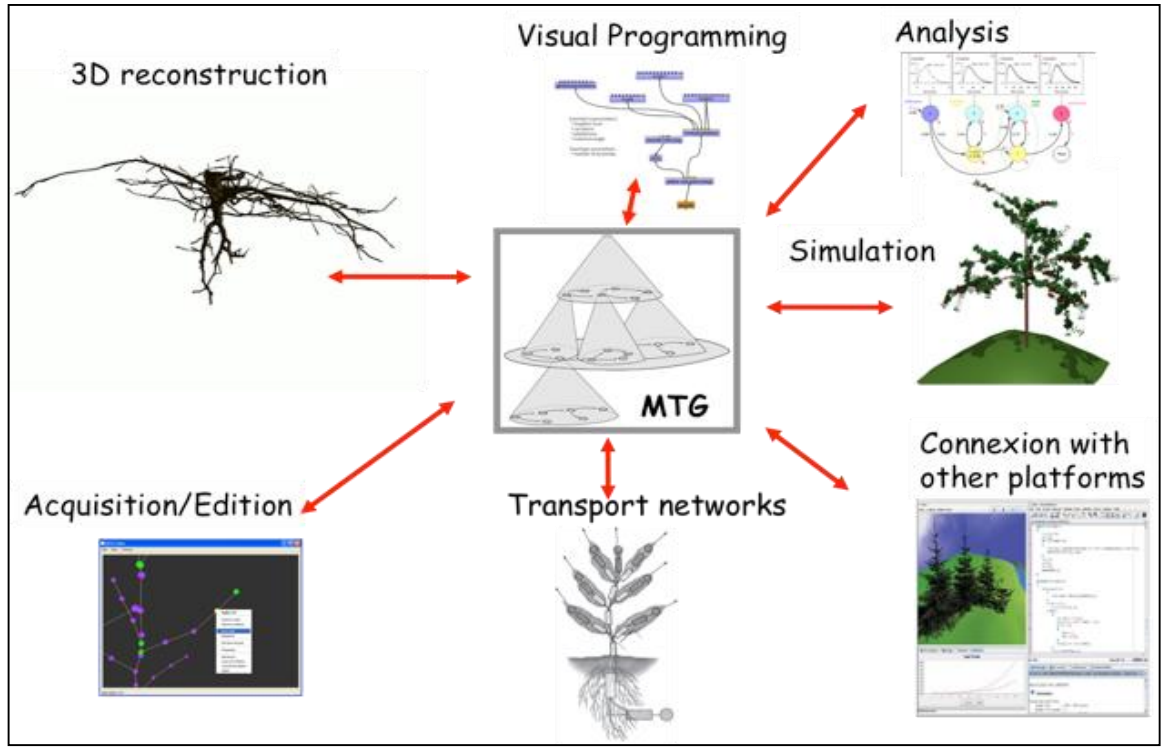


Open Source Community

- **Shared Governance**
  - CIRAD, INRAE, inria
- **Sharing models & formalisms**
  - Github, Conda, Jupyter, L-GPL

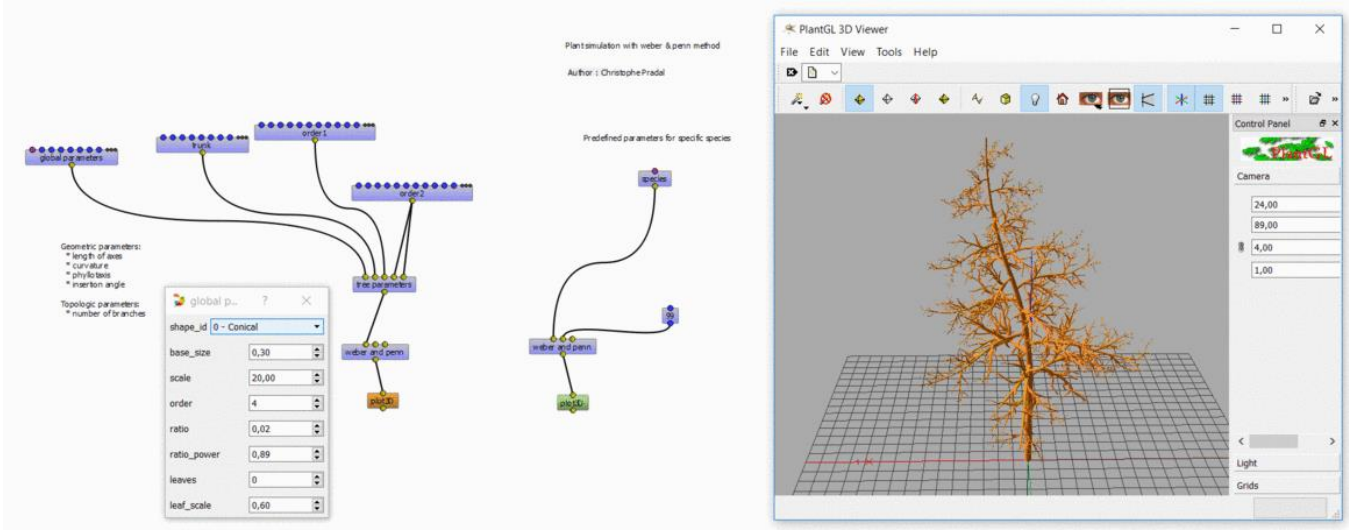
OpenAlea

- **Domains**
  - Plant modelling (FSPM)
  - Phenotyping
- **Solutions**
  - Integration framework
  - Shared Foundations (Math, CS)
  - Model repository & Modularity
  - Reproducible computational experiment



OpenAlea Design Principles

- Language Centric (Python)
  - Common Modelling Language
  - Glue Language
- Component Architecture
  - Dynamic composition
- Scientific Workflows
  - Visual Programming
  - Automatic GUI generation
  - Distributed Computation
- Virtual Research Environment
  - Jupyter Lab, Binder, Docker
- Shared Development Tools
  - Test, Doc, Versioning (git), CI, Deployment (conda)



Animation of the community

Modellers are not Computer Scientists!

Sprint

- Appear in OpenSource conferences (1st Hackathon OpenBSD 1999)
- Pair programming and Test Driven Development

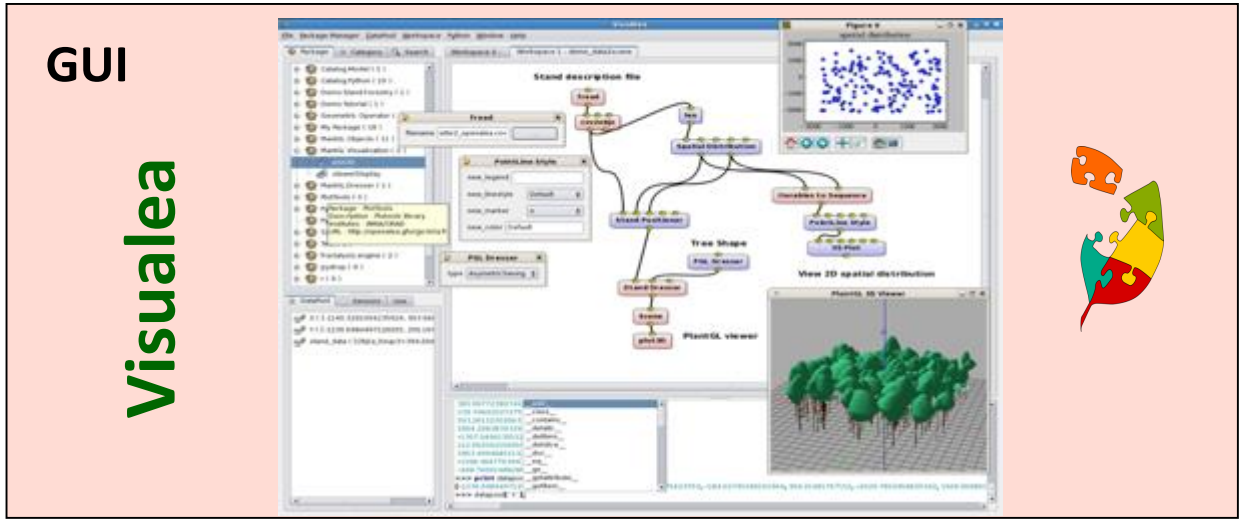
Coding Sprint

- Math & Computer Scientists
- Duration : 3 days, From 10 to 20 developers
- One cycle = One task = ½ day

Modelling Sprint

- Modellers
- Model integration and informal training
- Foster collaborations

OpenAlea Architecture

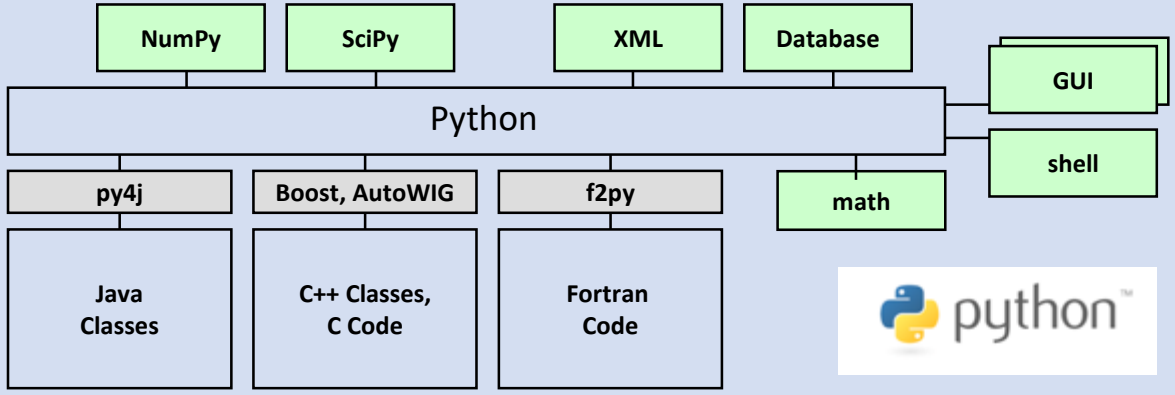


Component framework | Component | Package Manager | Scientific Workflows

Python Library

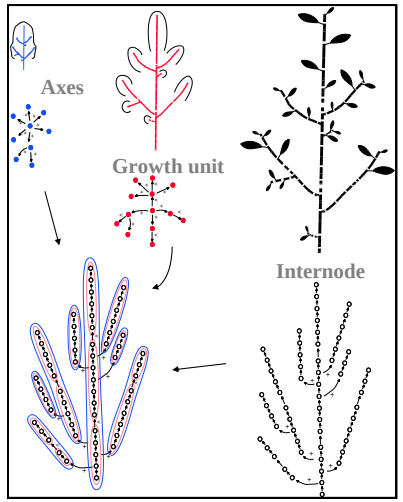
Existing Models

C, C++, Fortran, Java, R

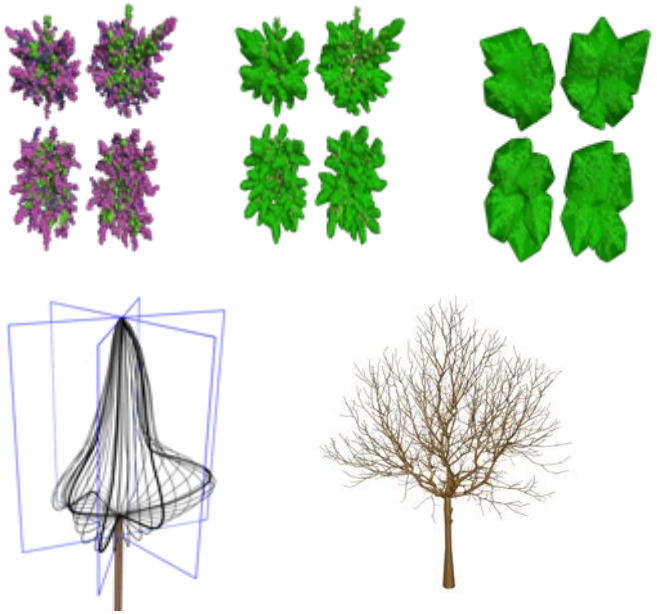


Formalisms in OpenAlea

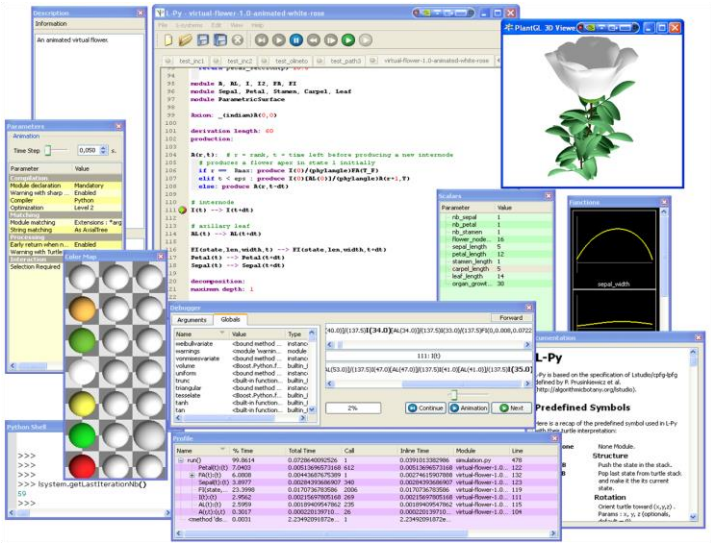
Multiscale **Topology** (MTG)
(Pradal, Godin)



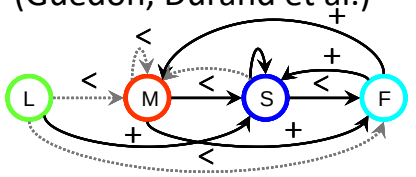
Multiscale **Geometry** (PlantGL)
(Boudon, Pradal et al.)

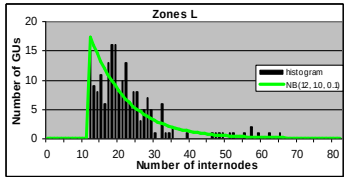


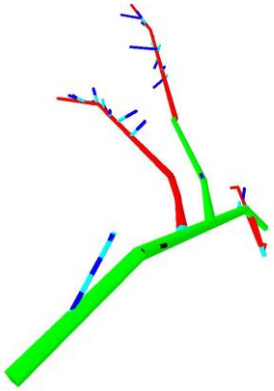
Simulation Framework (L-Py)
(Boudon et al., 2012)



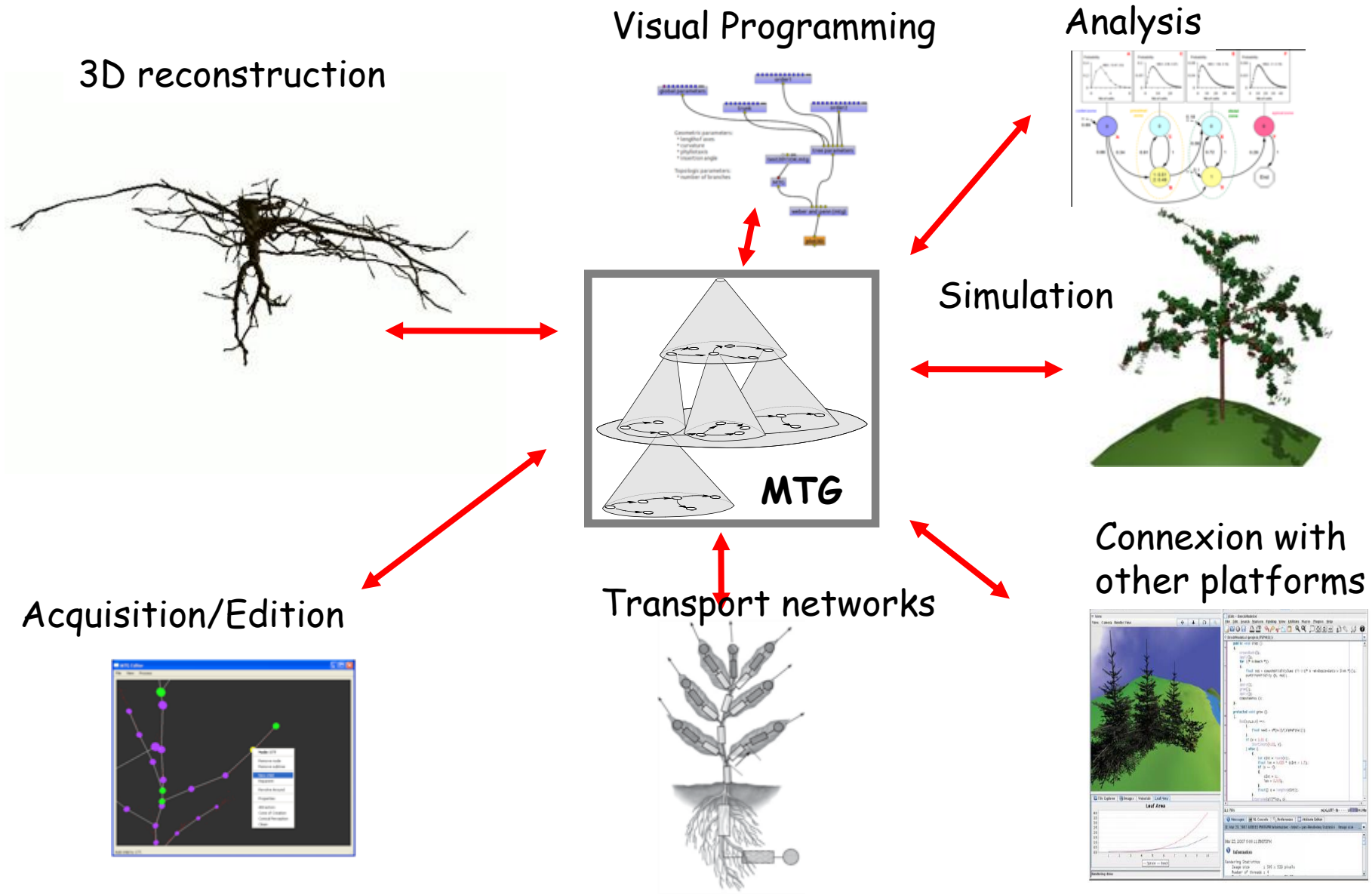
Statistical Structural Analysis
(Guédon, Durand et al.)







MTG as a central « blackboard »

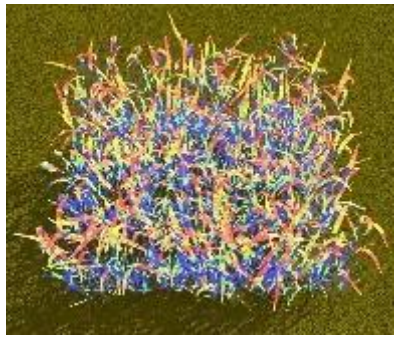


A catalog of Models as knowledge sources

Microclimate

(PIAF, Ecosys, LEPSE, AMAP)

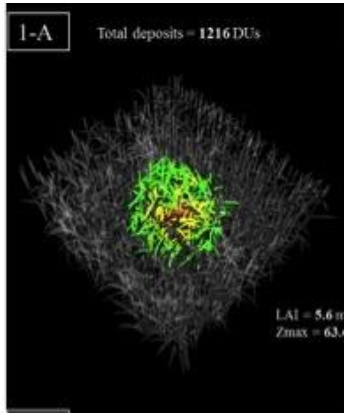
RATP, Caribu, Fractalysis

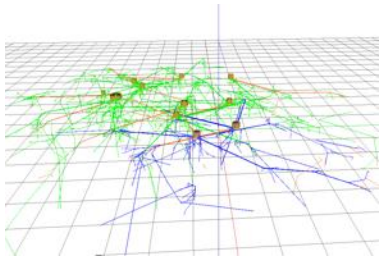


Plant / Pathogen

(Ecosys, LEPSE, AGAP, itk)

Septo3D, Alep, ECHAP



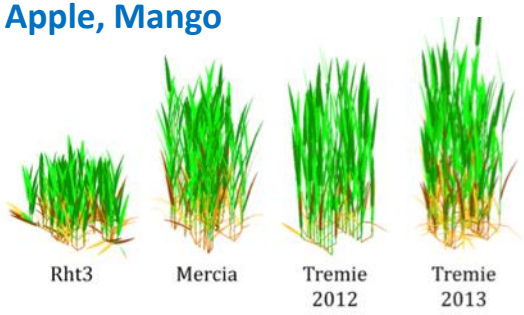


Architectural models

(LEPSE, AGAP, U3PF, ECOSYS, HortSys)

Adel (wheat, Maize), Pea, Vine, Strawberry

Apple, Mango

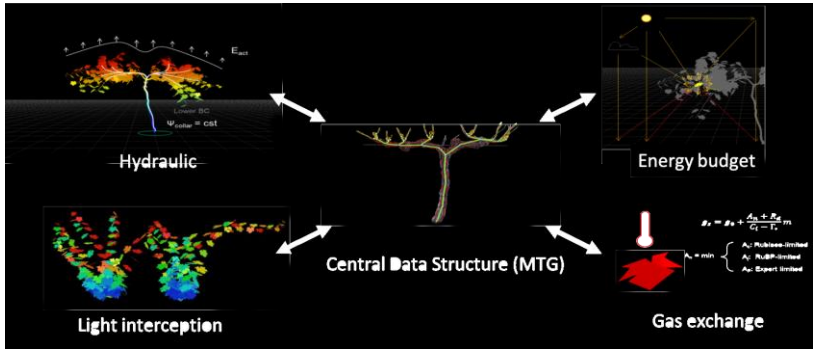


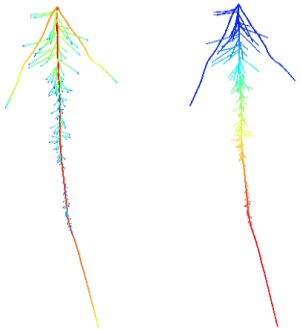
Plant Functions

(BPMP, LEPSE, AGAP, U3PF, ECOSYS, DIADE)

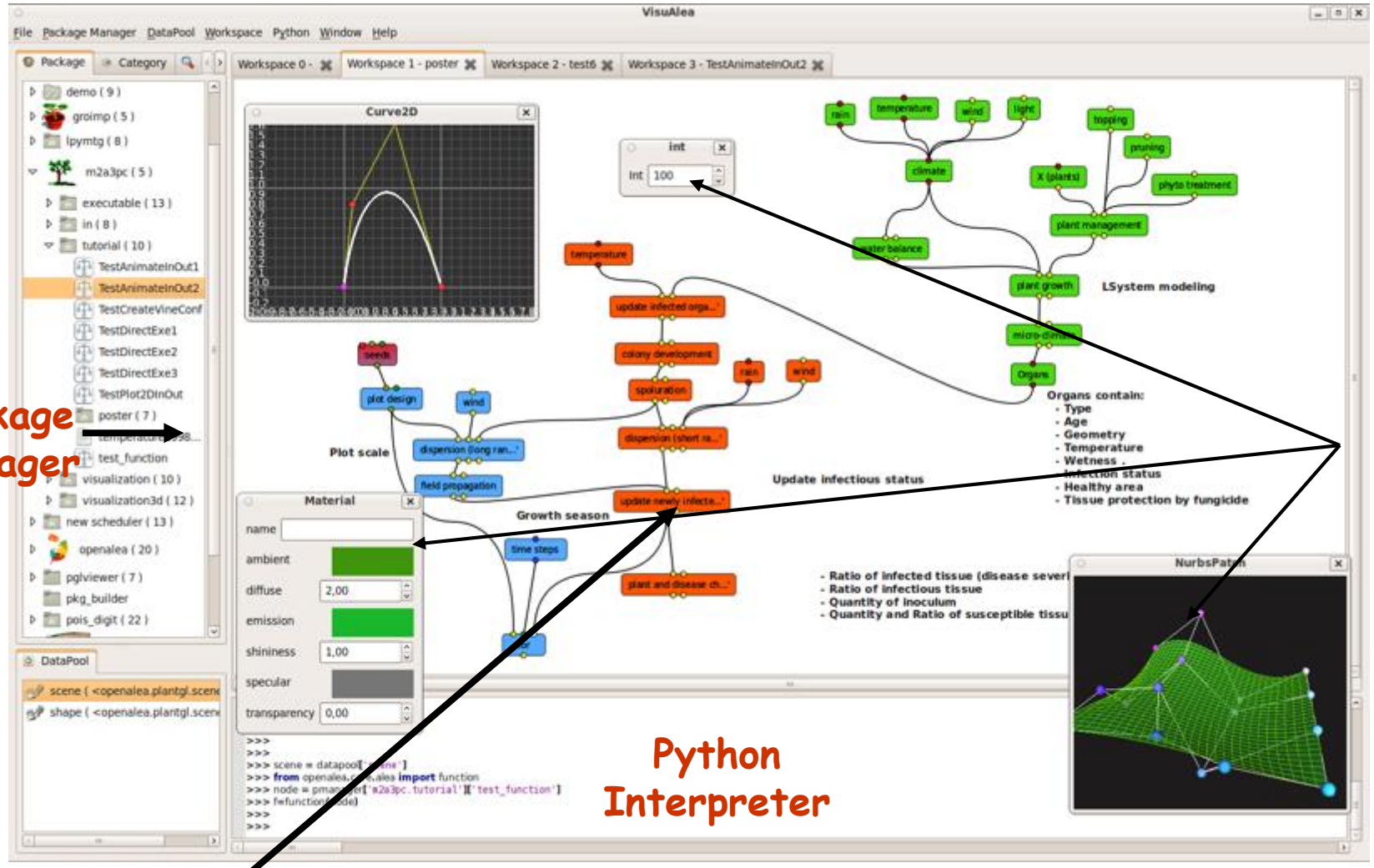
C, N, Photosynthesis, Hydraulic

CN-Wheat, HydroShoot, HydroRoot, …





Visual Programming & Scientific Workflows



Scientific Workflows (swf) : ASAP

Automation

- swf to automate computational aspects of science

Scaling (exploit and **optimize** machine cycles)

- swf should make use of **parallel compute resources**
- swf should be able handle **large data set**

Abstraction, Evolution, Reuse (human cycles)

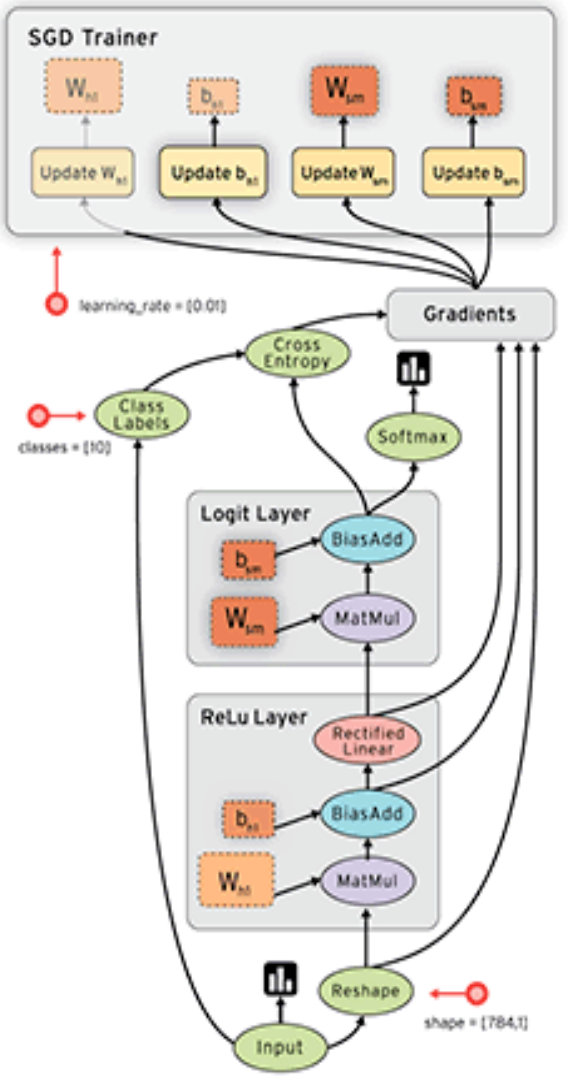
- swf should be easy to (re-)use, evolve, share

Provenance

- swf should capture **processing history**, **data lineage**

  -> traceable data- and wf- evolution

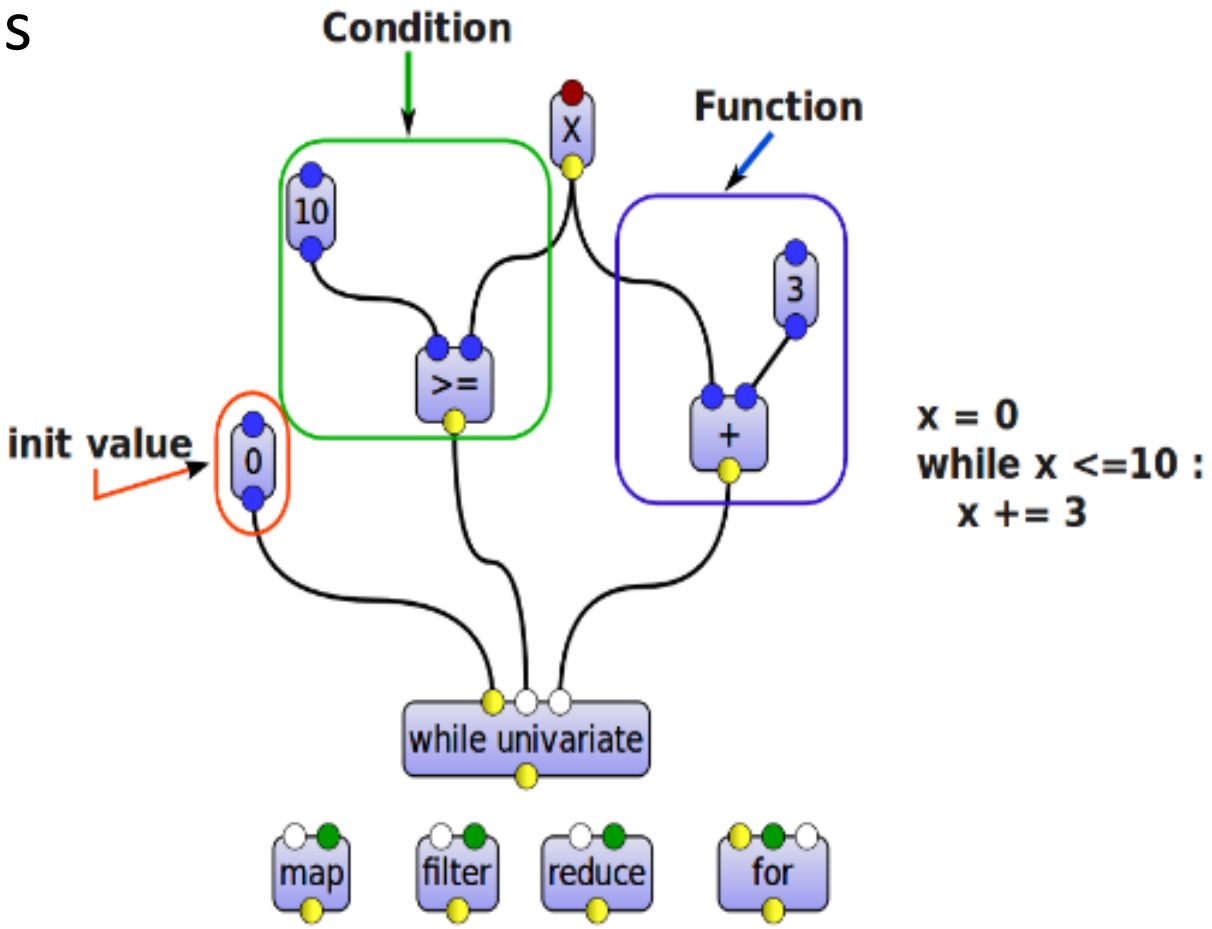
Cuevas *et al.*, 2012



Tensorflow, Abadie/google, 16

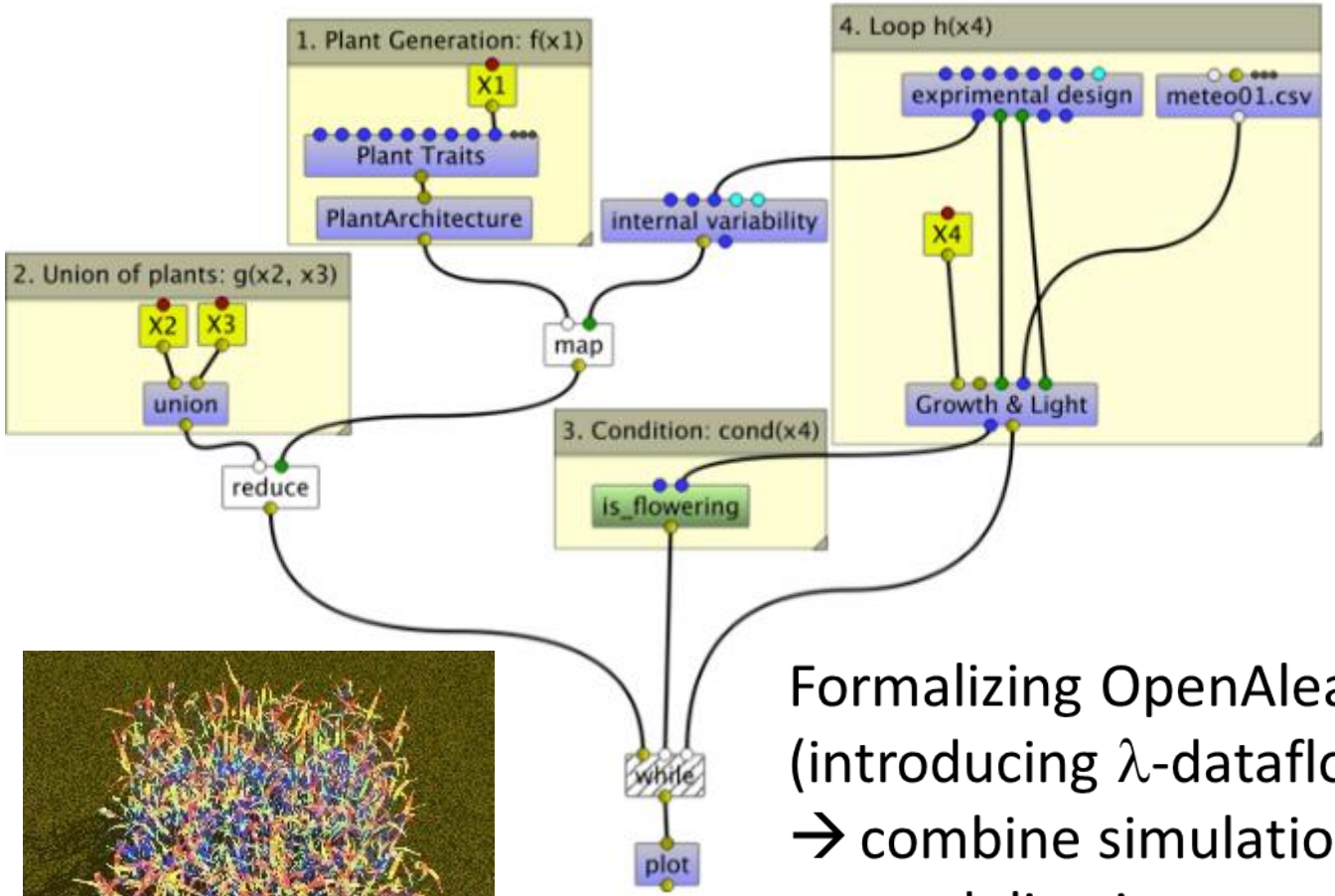
Algebraic Scientific Workflows

- Control-flow using lambda-calculus
- Dataflow Variable (X)
  - Transform a dataflow into a function
- Algebraic Operator
  map, reduce, filter…



Pradal, Fournier, Valduriez, Cohen-Boulakia. SSDBM 2015

Higher-order Scientific Workflows



Formalizing OpenAlea workflows (introducing λ-dataflow)

→ combine simulation and modelisation

→ express retroaction loops

Pradal, Fournier, Valduriez, Cohen-Boulakia. SSDBM 2015

Outline

- OpenAlea software platform
- **HTP Shoot Phenotyping & Modelling**
- HTP Root Architecture & Modelling
- Crop modelling framework interoperability

HTP Platforms (Phenoarch - Montpellier)

Cabrera-Bosquet et al. 2016 New Phytologist

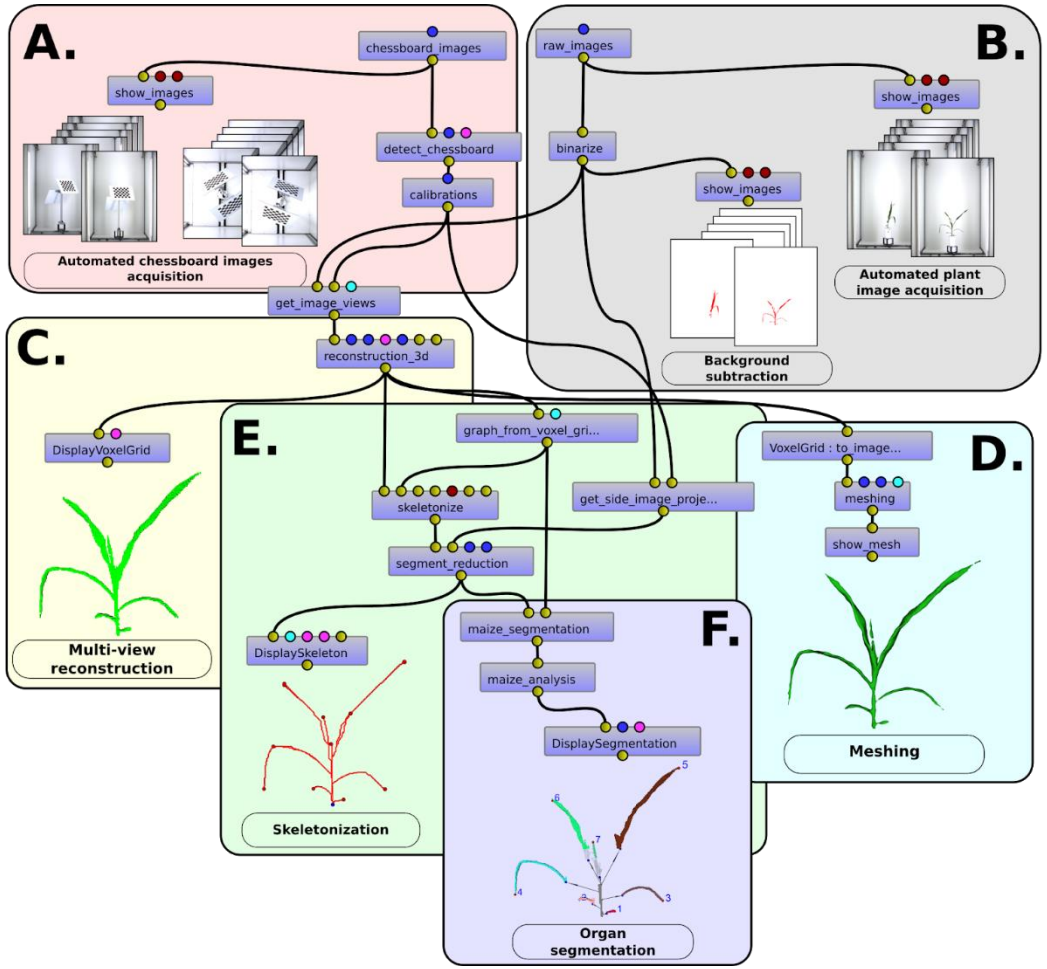
Analyses of **genetic determinisms** of plant **responses to environmental conditions** (drought, temperature and light)

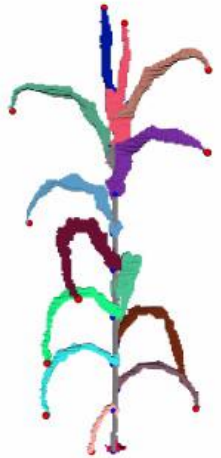
- Capacity for **2400** plants (ca. 300 genotypes)
- Automated trait measurements

Symbols	Units	Traits	Type of area distribution
LA	m^2	Plant leaf area	-
h_{stem}	cm	Stem height	vertical
θ	degrees	Plant inclination index	vertical & horizontal
rh_{PAD}	-	Plant relative height where half plant leaf area is reached	vertical
b_{PAD}	-	Distribution of leaf area along plant height	vertical
radius	cm	Plant radius	horizontal & vertical
σ_{az}	degrees	azimuths dispersion	horizontal
Δ_{row}	degrees	azimuth deviation from row	horizontal

M3P Montpellier Plant Phenotyping Platforms

Phenomenal: an automatic image analysis workflow



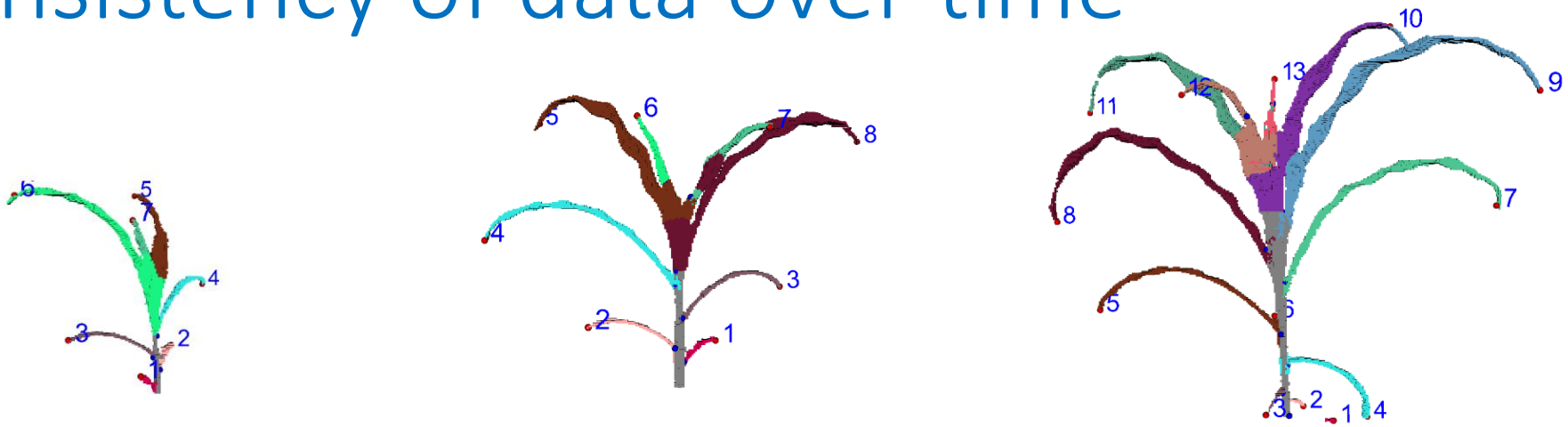


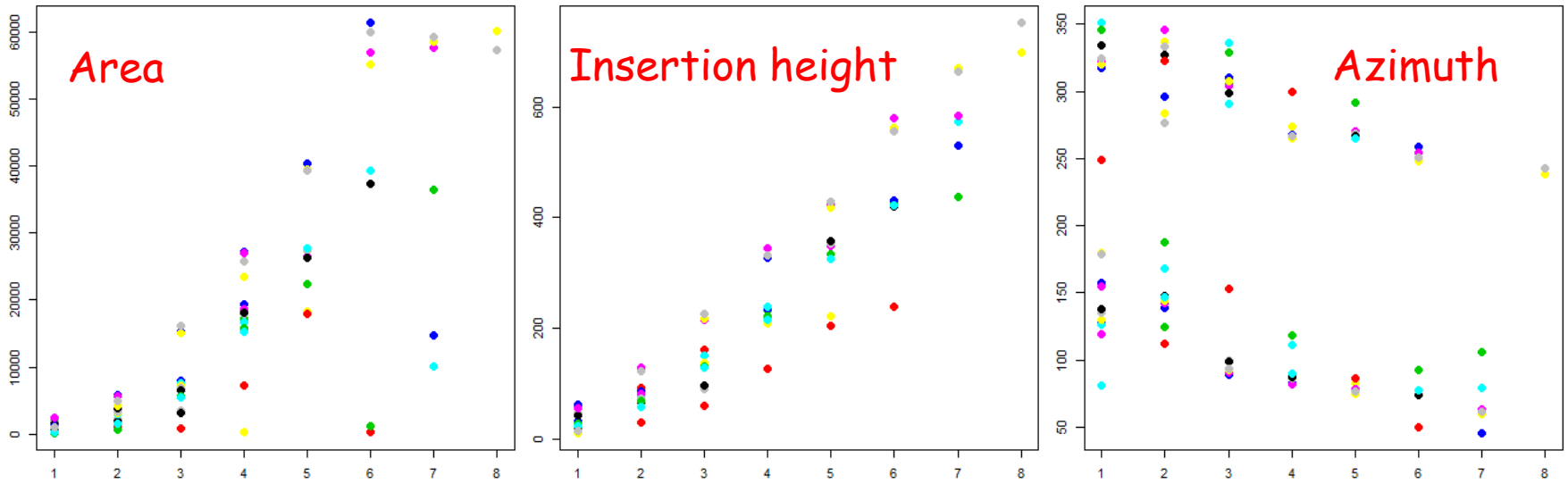
OpenAlea

PHENOME EMPHASIS

https://github.com/openalea/phenomenal

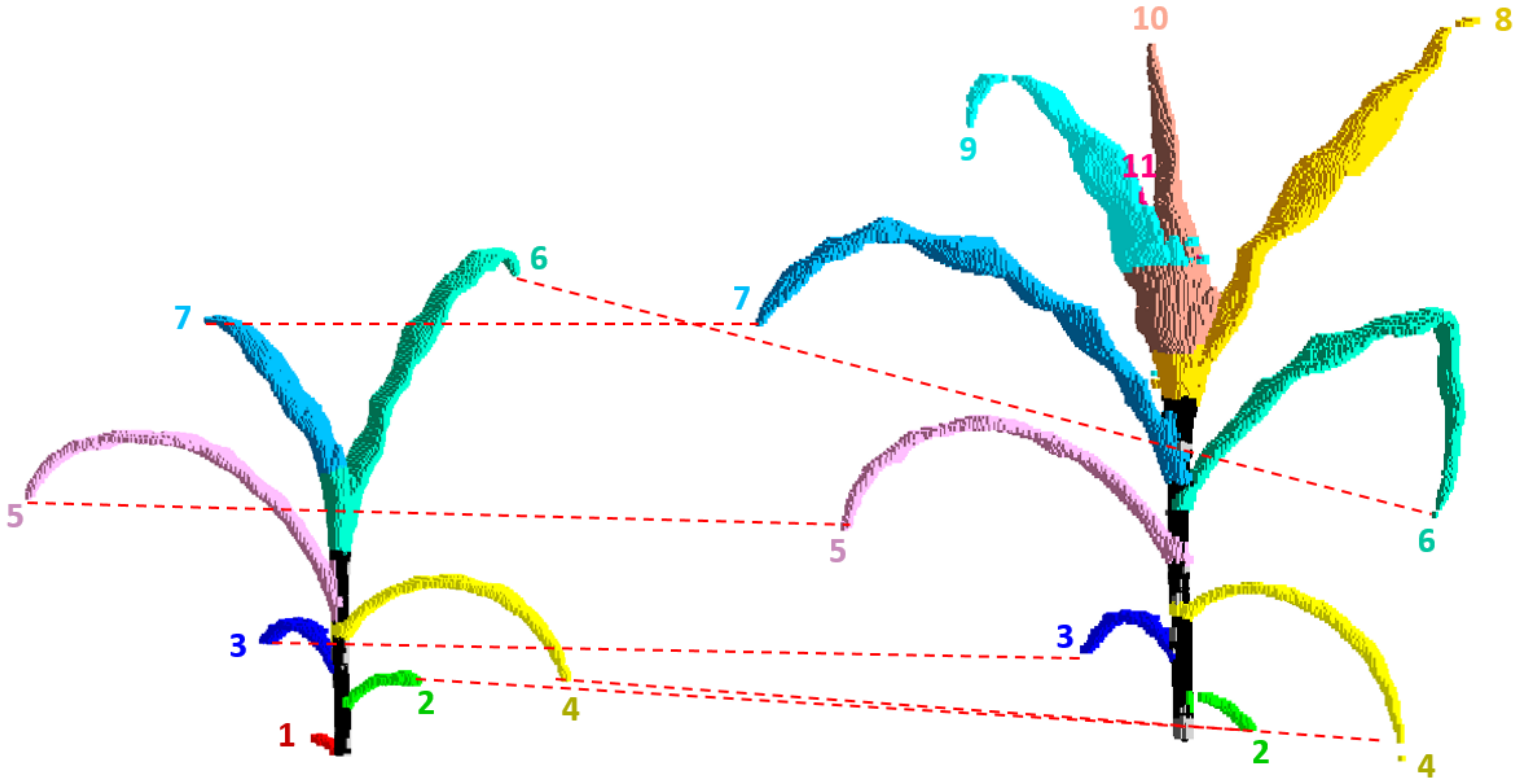
Inconsistency of data over time





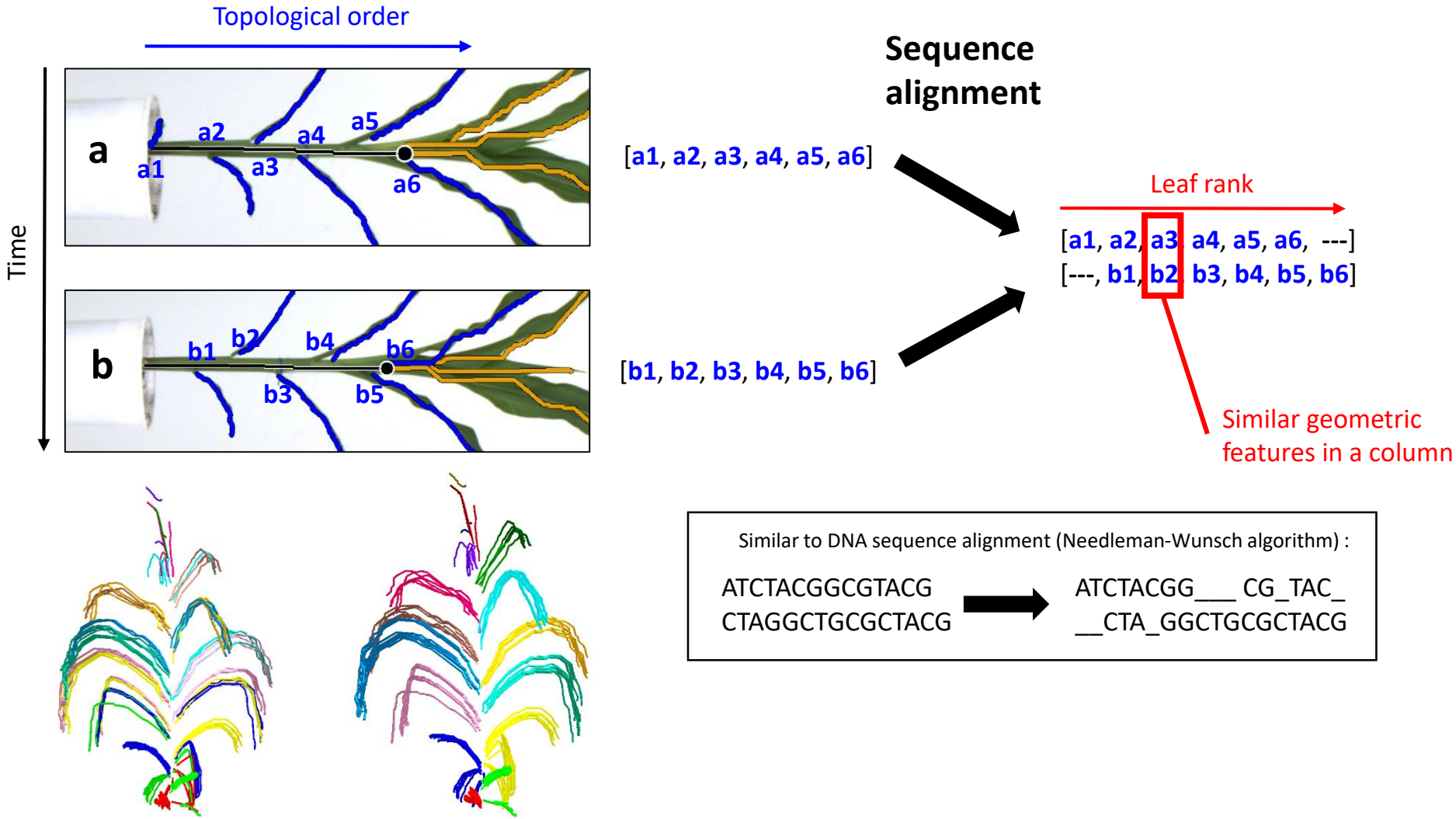
Leaf Position

Solution: Tracking

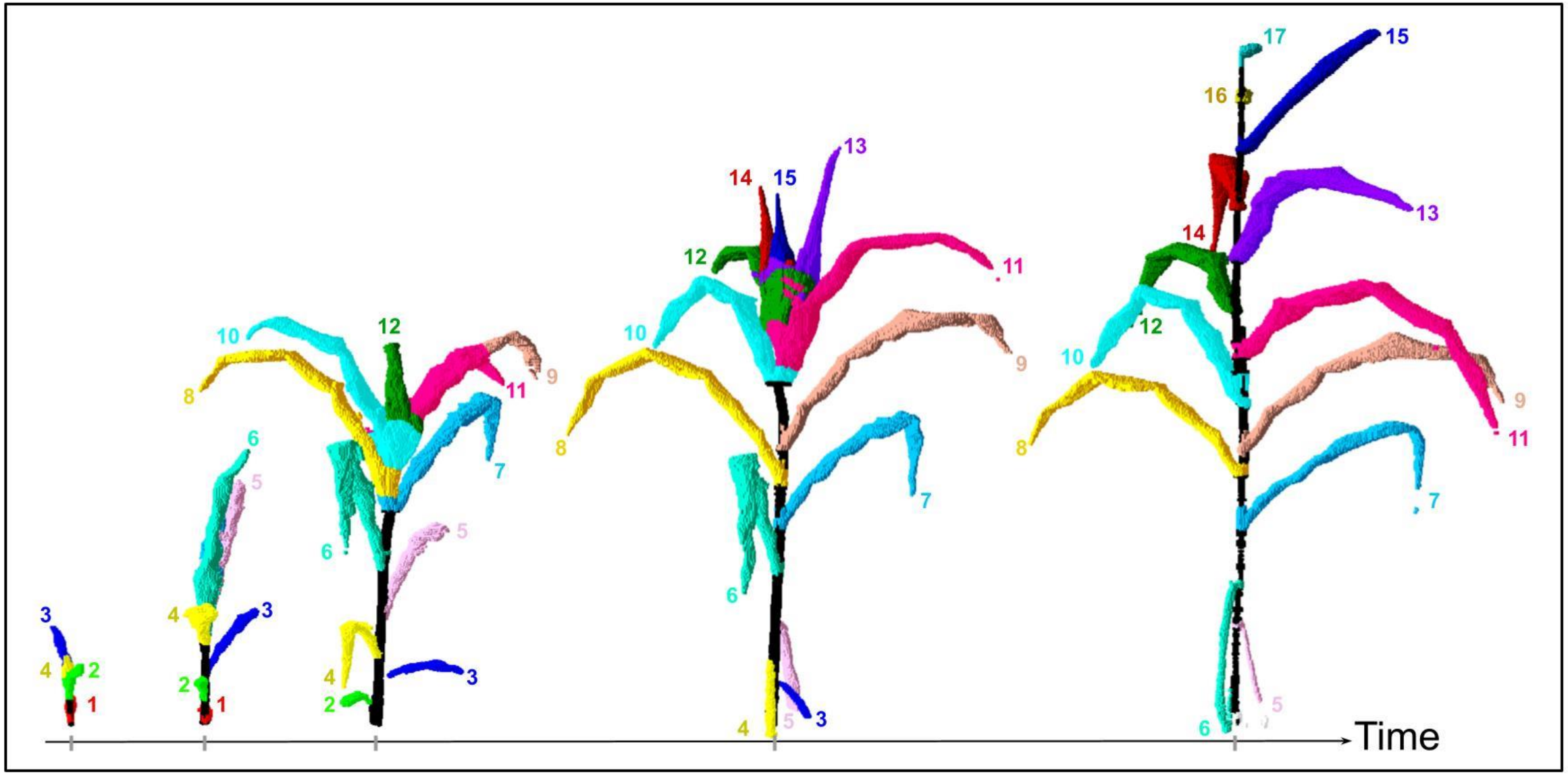


Daviet, Fernandez et al., Plant Methods, in rev.

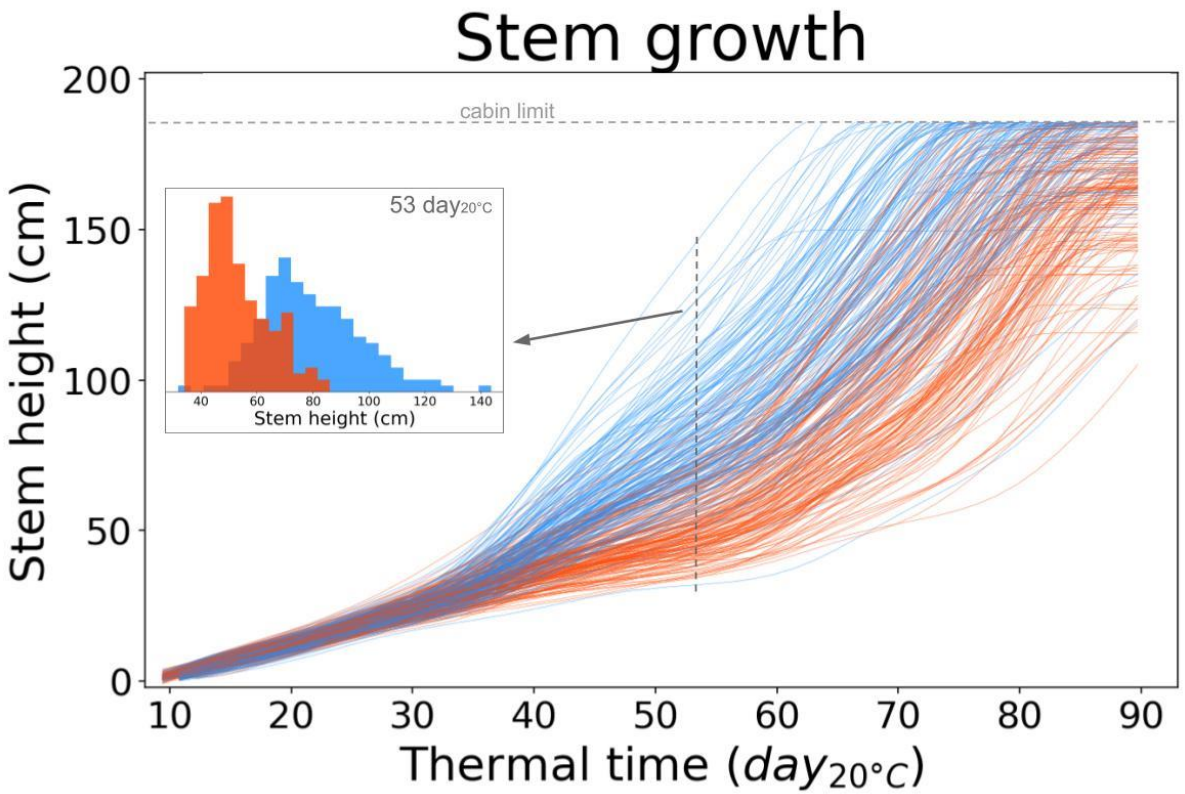
Tracking mature leaves as a multiple sequence alignment problem

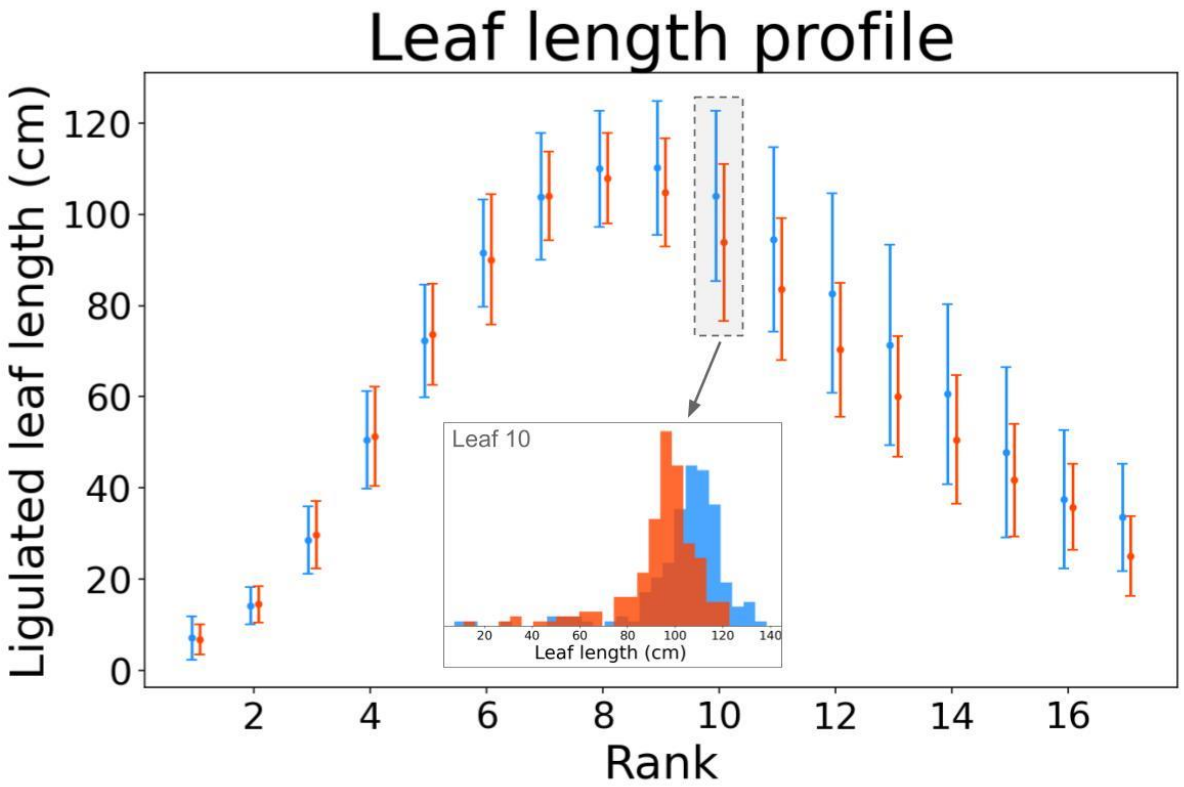


Tracking organs over time



Automatic HT Measurements of traits

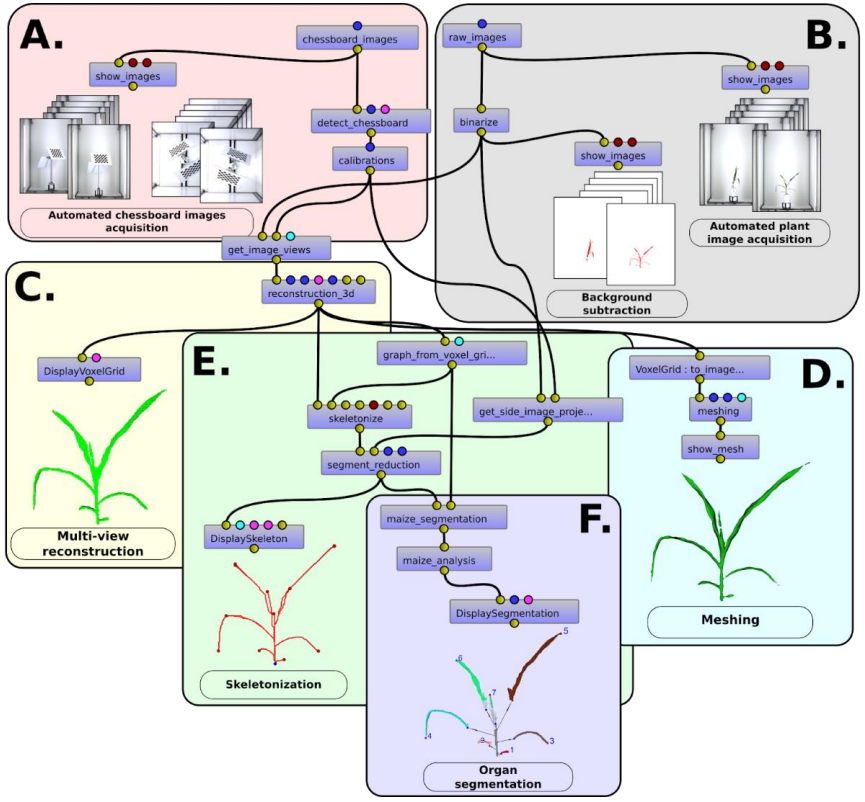


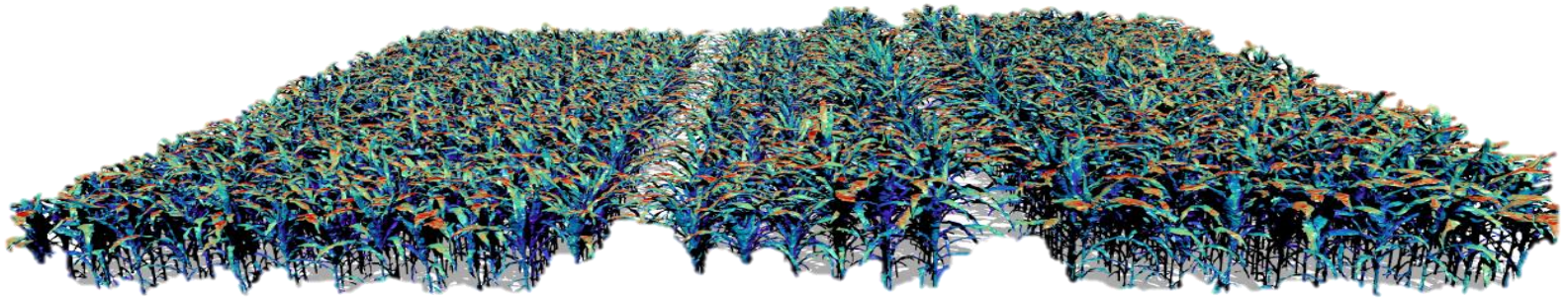


355 plants / 60 Genotypes x 42 dates under WW (blue) & WD (red)
237 K images analysed

Predicting state-variables by simulation

Estimating Light interception efficiency on a reconstructed canopy





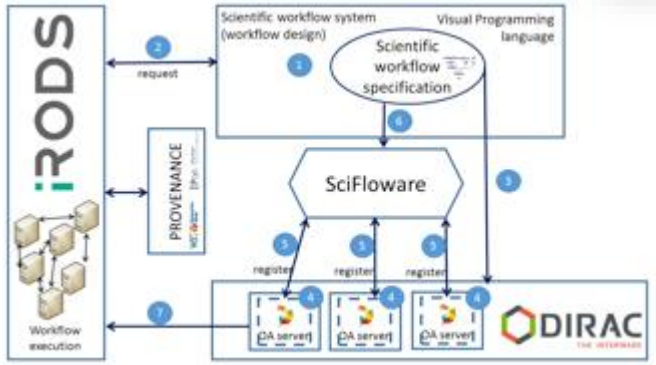
Cabrera-Bosquet et al. 2016 New Phytol.
Artzet et al., Plant Physiol., in rev.

Plant Phenomics and Distributed Computing

- Coupling HTP analysis with biophysical models using Scientific Workflows

PhenoArch, LEPSE, Montpellier

→ Higher-order Scientific Workflows
→ Enhancing reproducibility (provenance)



→ **InfraPhenoGrid**: An infrastructure for Phenotyping on the Grid
→ **OpenAlea.Phenomenal**: automatic 3D shoot reconstruction

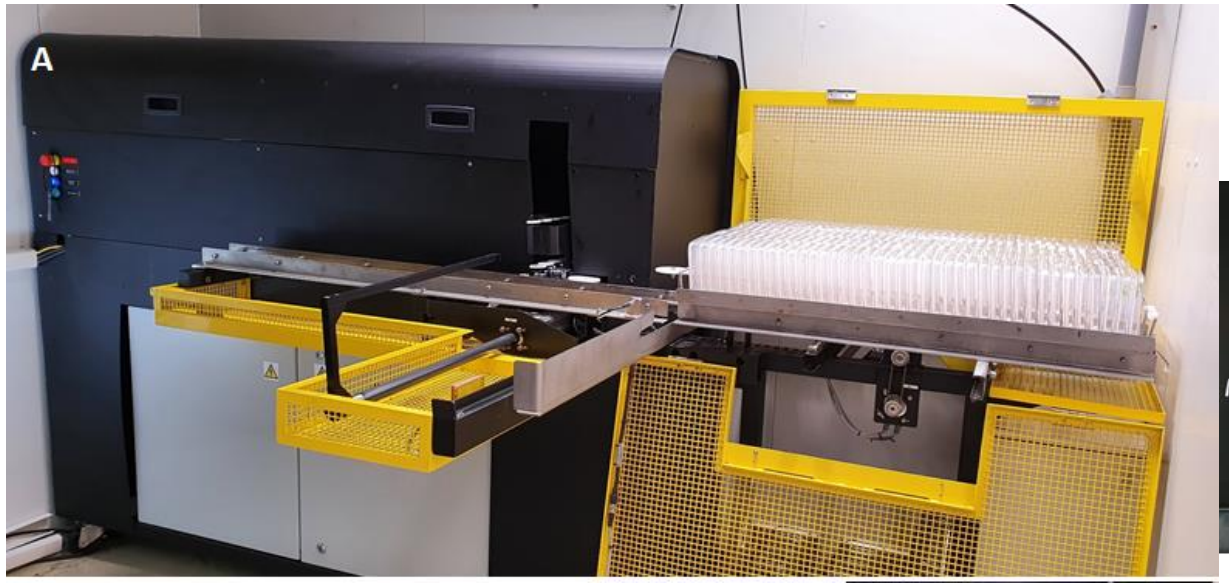
→ Grid & Cloud computing using OpenAlea

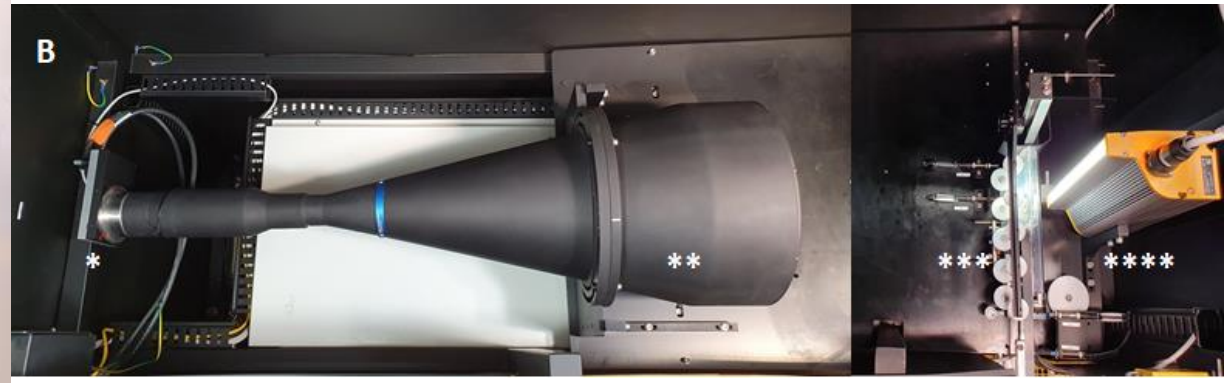
Pradal et al., 2017. FGCS InfraPhenoGrid
Heidsieck et al., 2021, FGCS

Outline

- OpenAlea software platform
- HTP Shoot Phenotyping & Modelling
- **HTP Root Architecture & Modelling**
- Crop modelling framework interoperability

Time-lapse tracking and reconstruction of root system architecture





HIgh Resolution ROot Scanner (HIRROS) setup for automated and non-destructive visualization of root architecture of seedlings grown in agar plates

IPSIM Montpellier

P. Nacry / INRAe

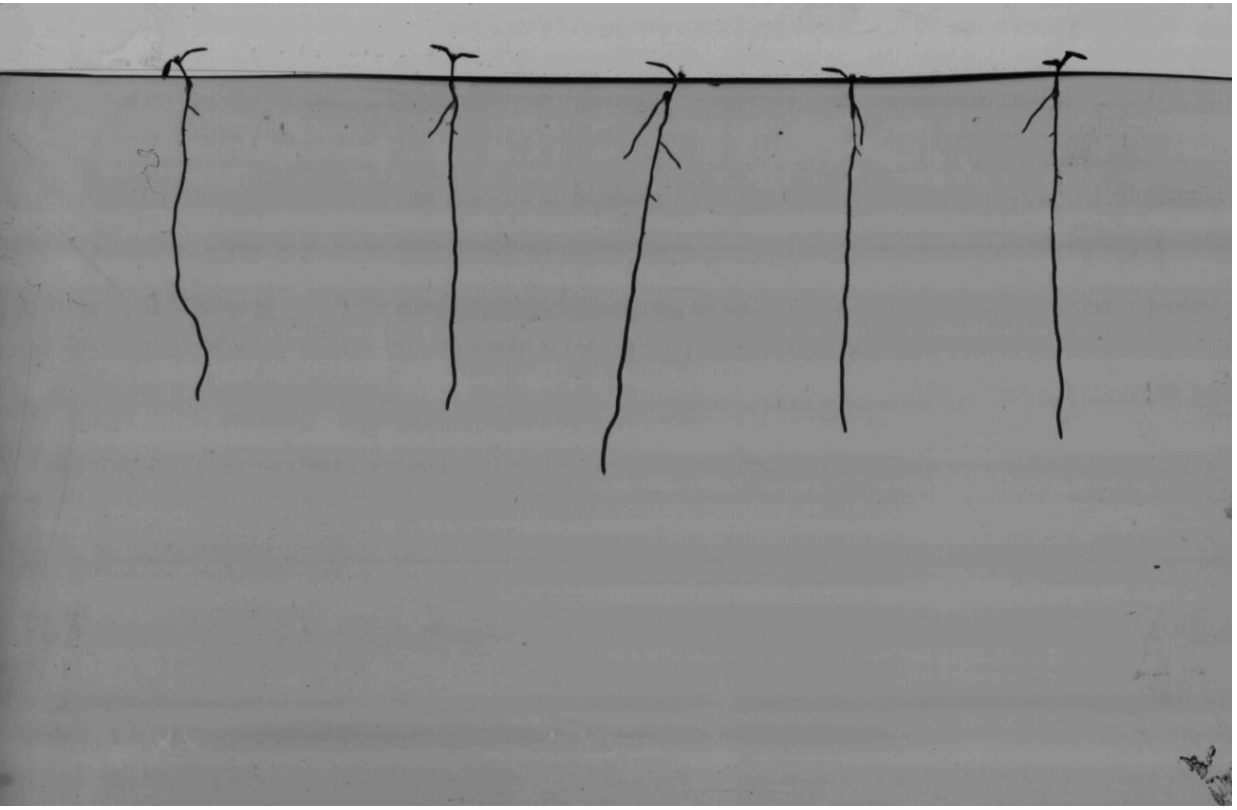
Fernandez et al., *Plant Methods, in rev.*

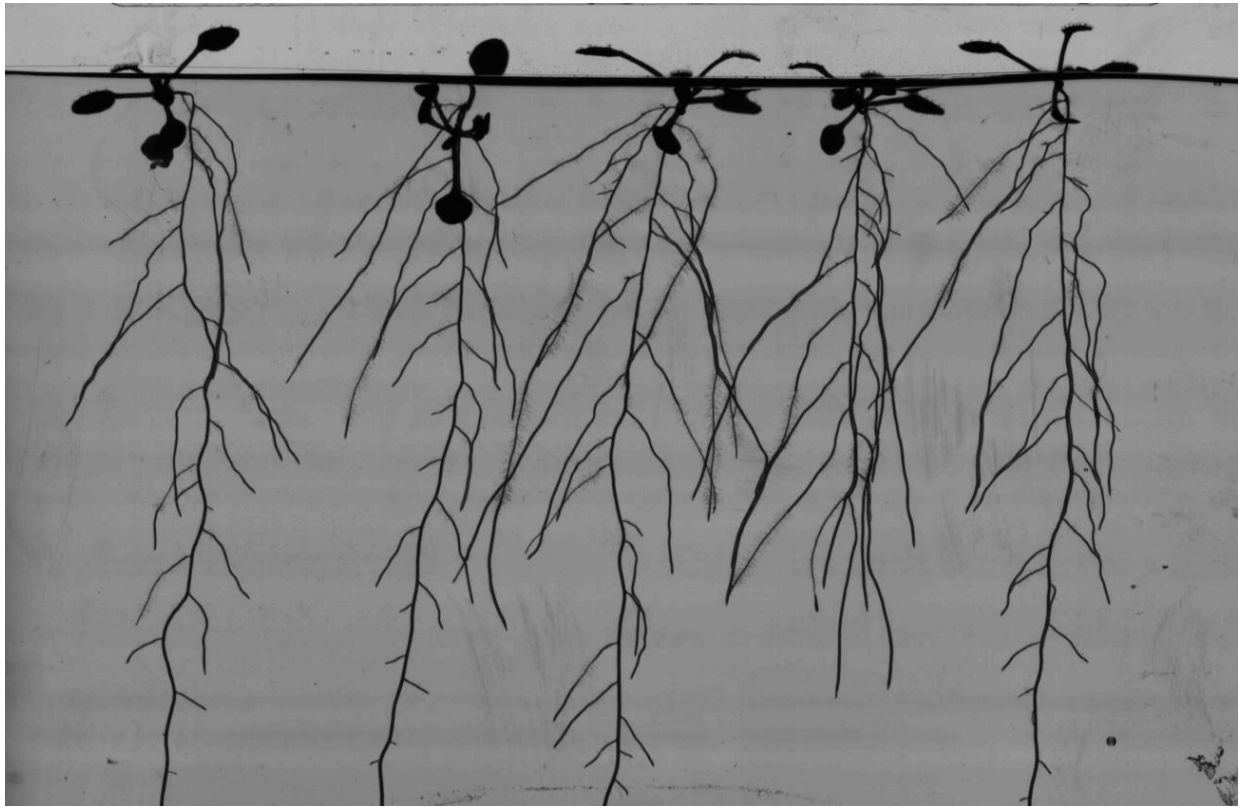
Phenotyping root systems

→Imaging robots

→ Possibility of time-lapse tracking

Automatic phenes extraction





?

Topological tracking: intuition

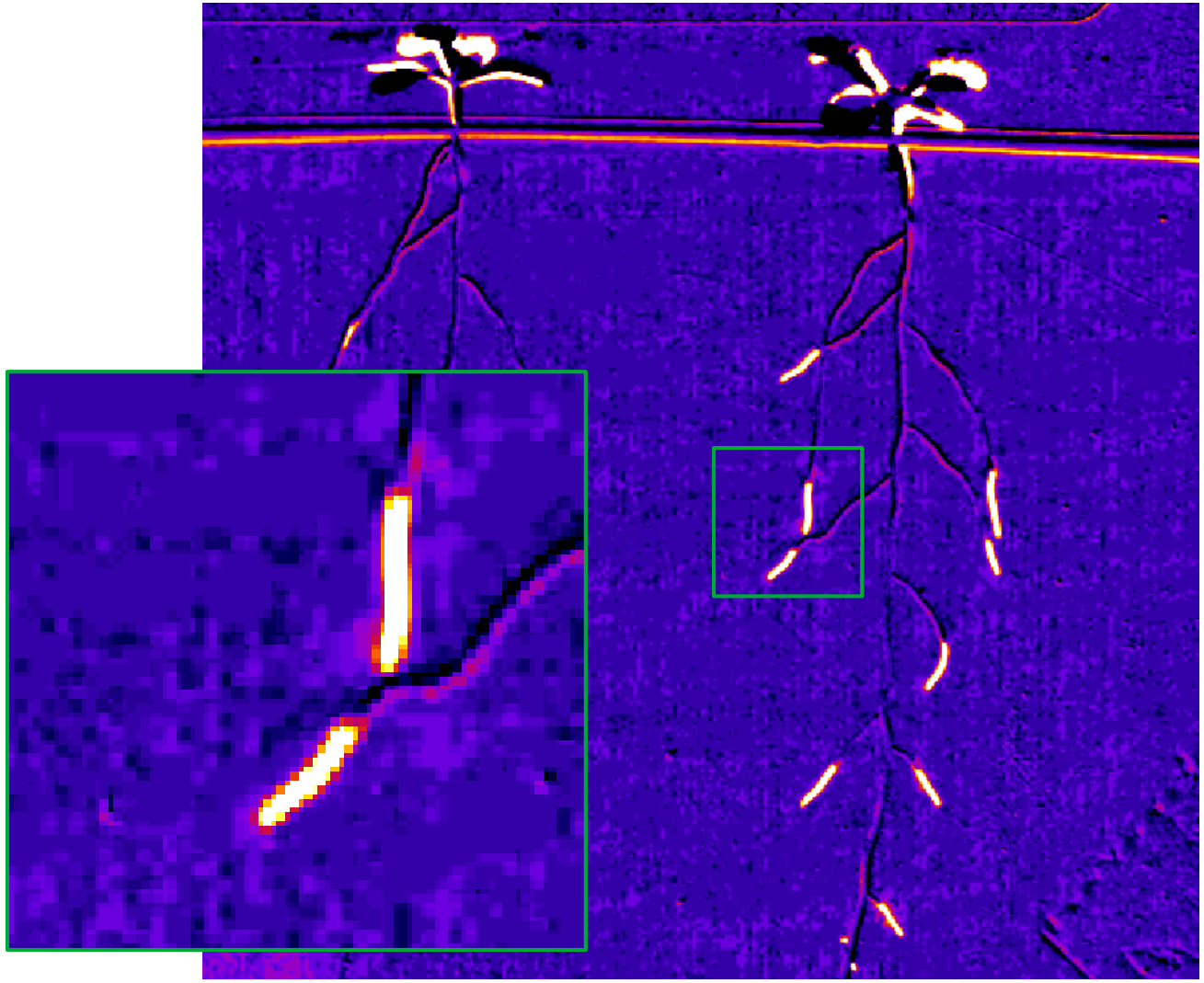
Complexity emerge...
time after time

△t => △roots

Topological tracking: intuition

Complexity emerge...
time after time

△t => △roots

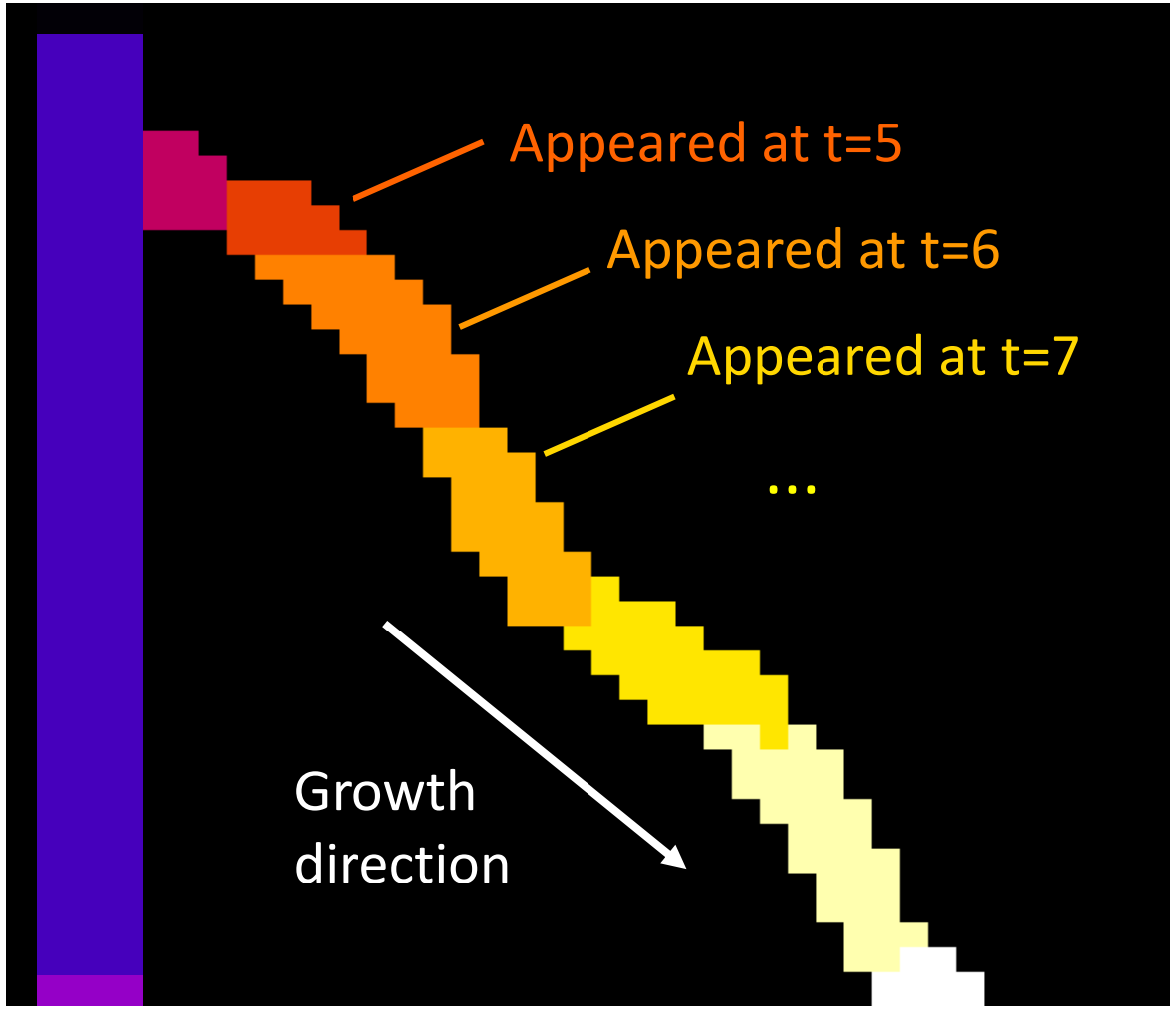


Difference between two successive images

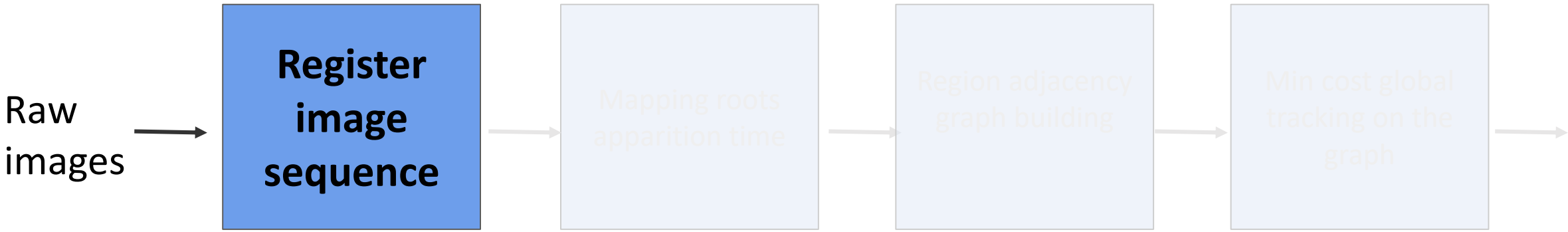
Topological tracking: intuition

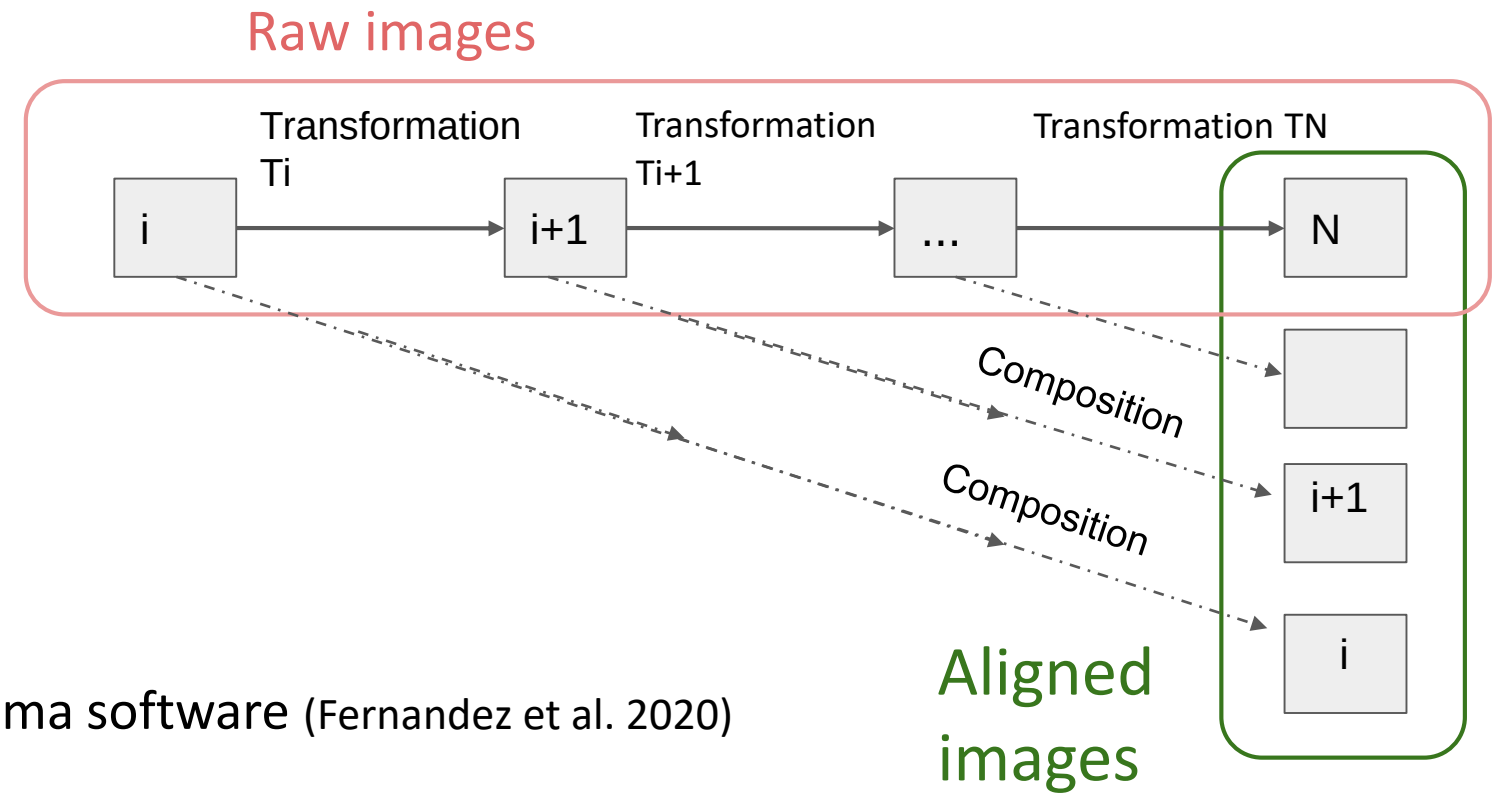
Complexity emerge...
time after time

△t => △roots



Topological tracking pipeline

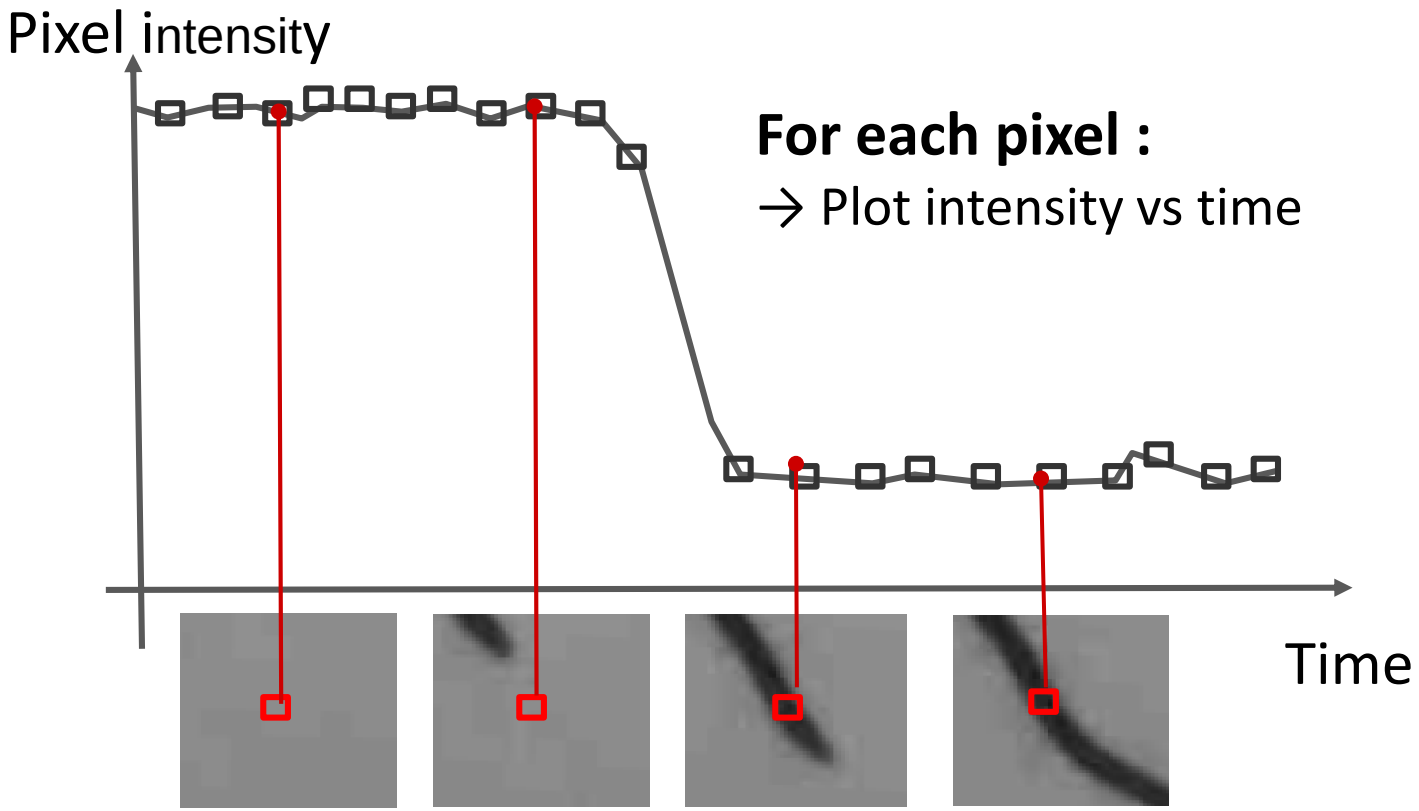




Daisy-chain registration through Fijiyama software (Fernandez et al. 2020)

Topological tracking pipeline

Raw images → Register image sequence → **Mapping roots apparition time** → Region adjacency graph building → Min cost global tracking on the graph

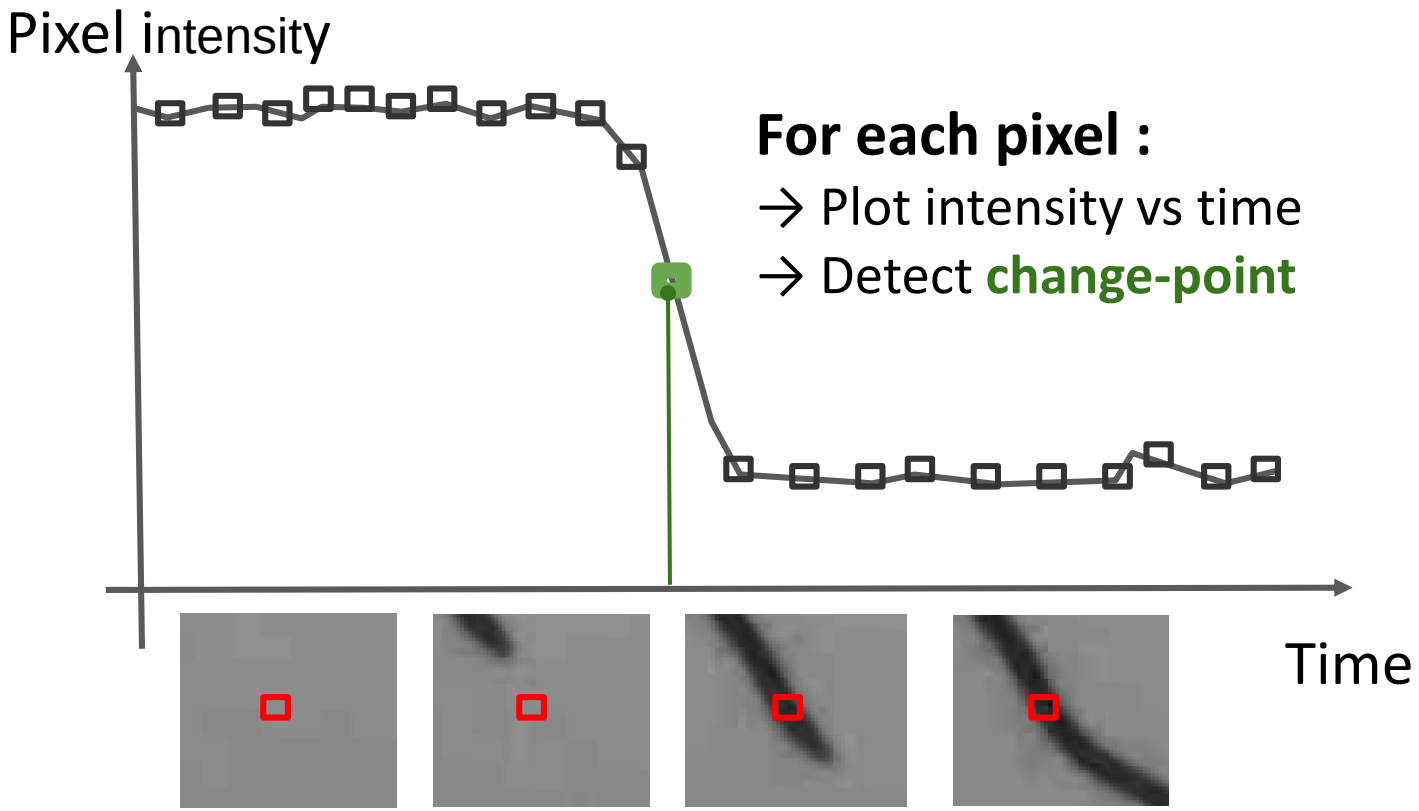


For each pixel :

→ Plot intensity vs time

Topological tracking pipeline

Raw images → Register image sequence → **Mapping roots apparition time** → Region adjacency graph building → Min cost global tracking on the graph

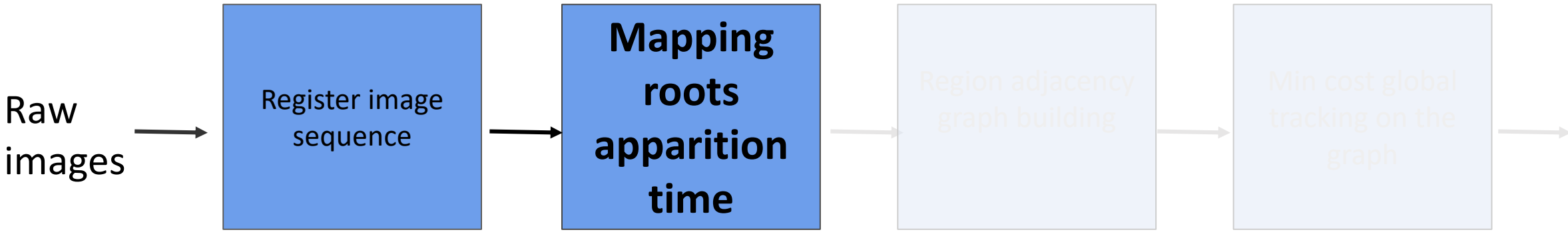


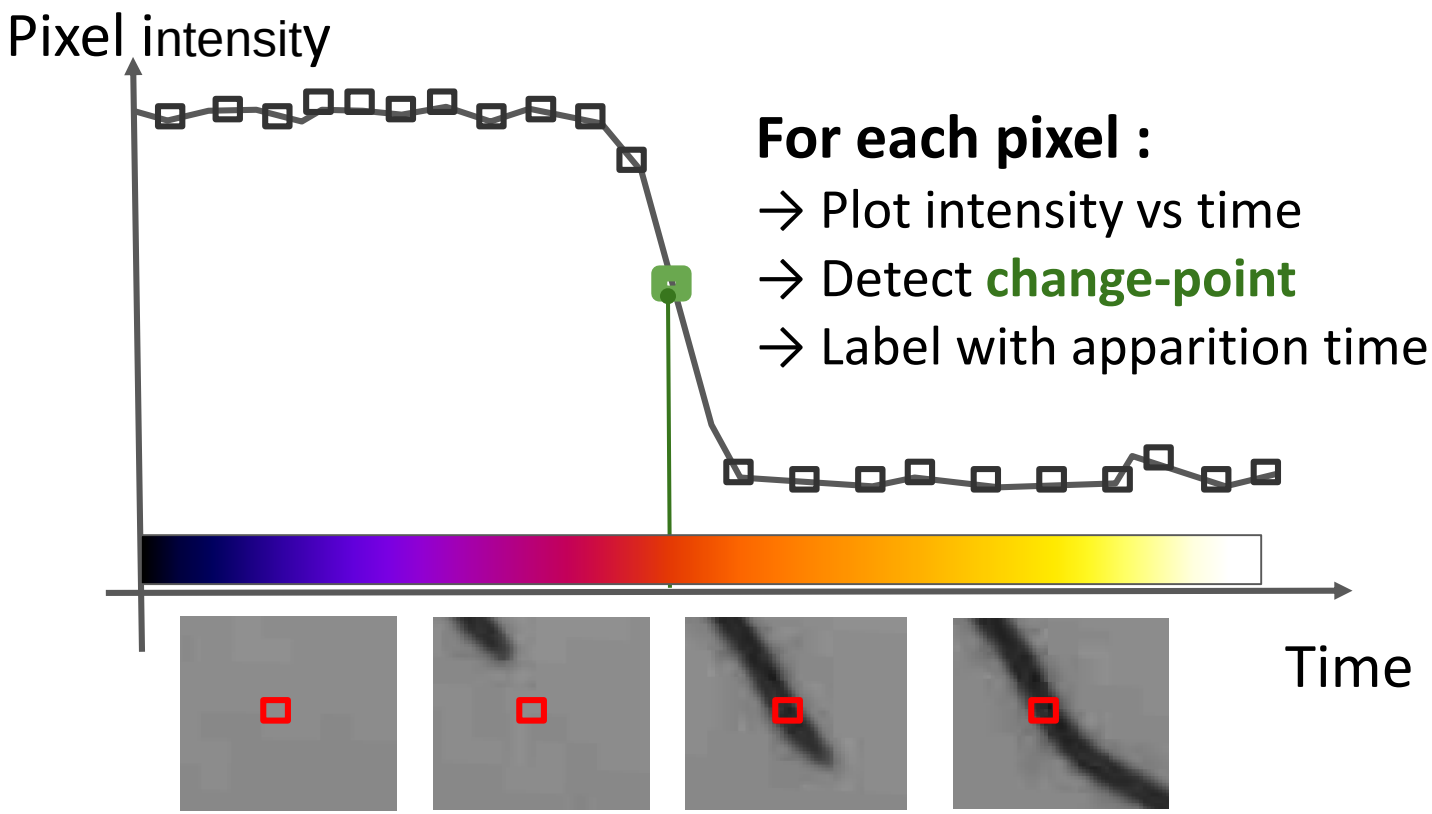
For each pixel :

→ Plot intensity vs time

→ Detect **change-point**

Topological tracking pipeline



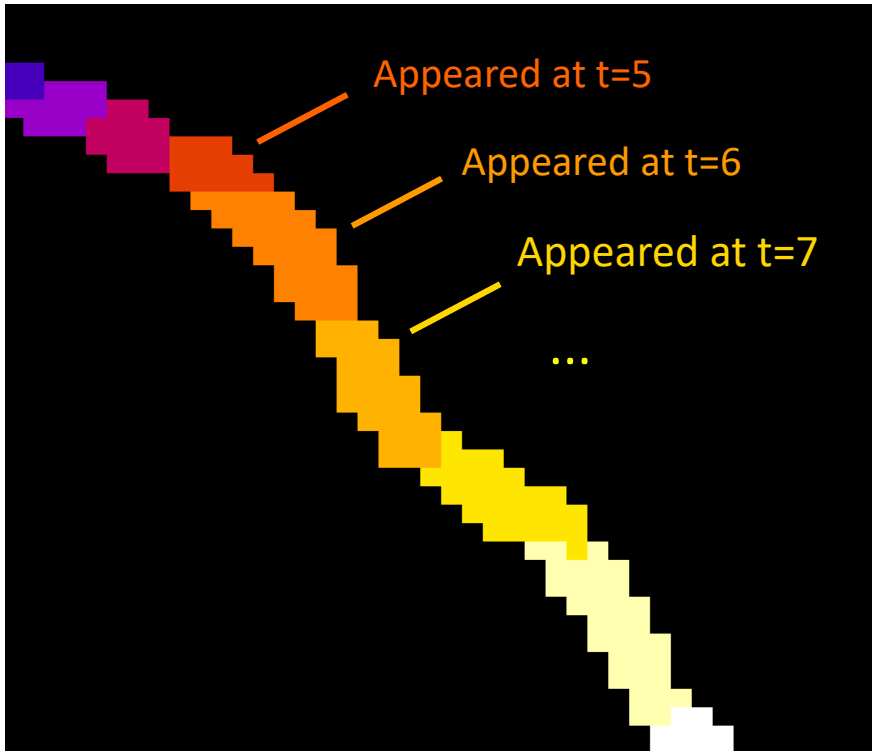


For each pixel :

→ Plot intensity vs time

→ Detect **change-point**

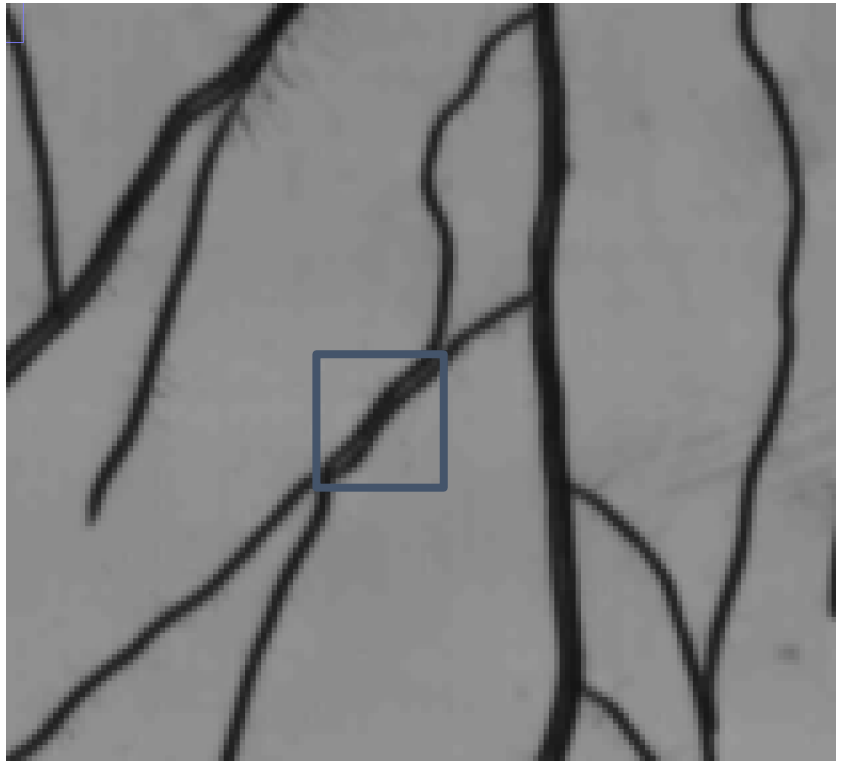
→ Label with apparition time

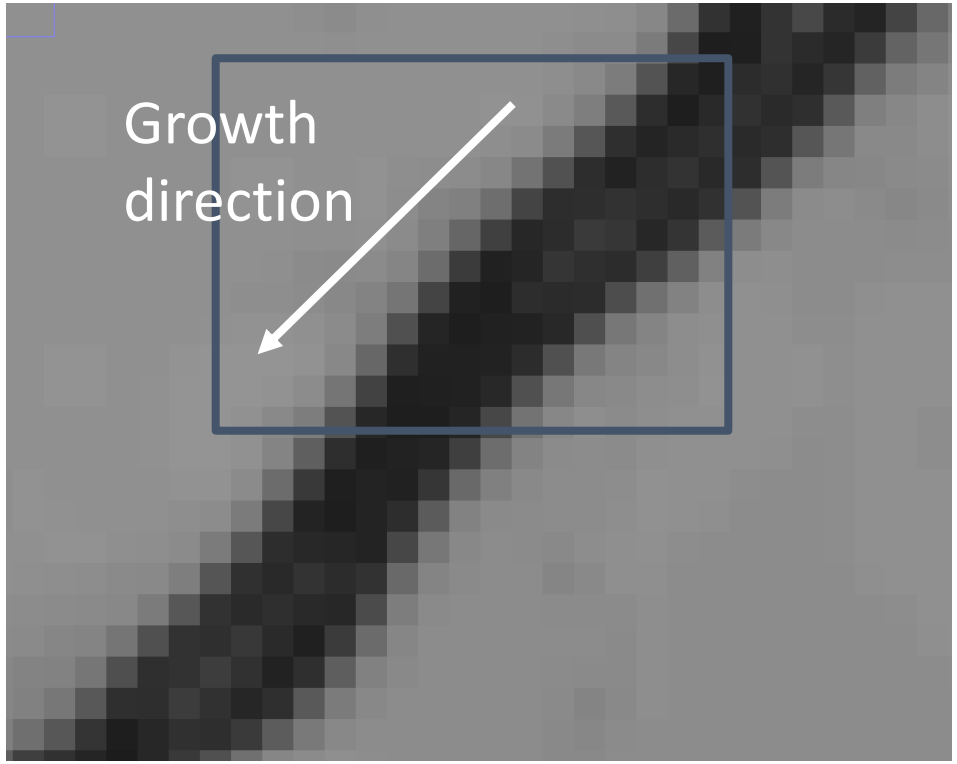


Pixel-wise date map

Topological tracking pipeline

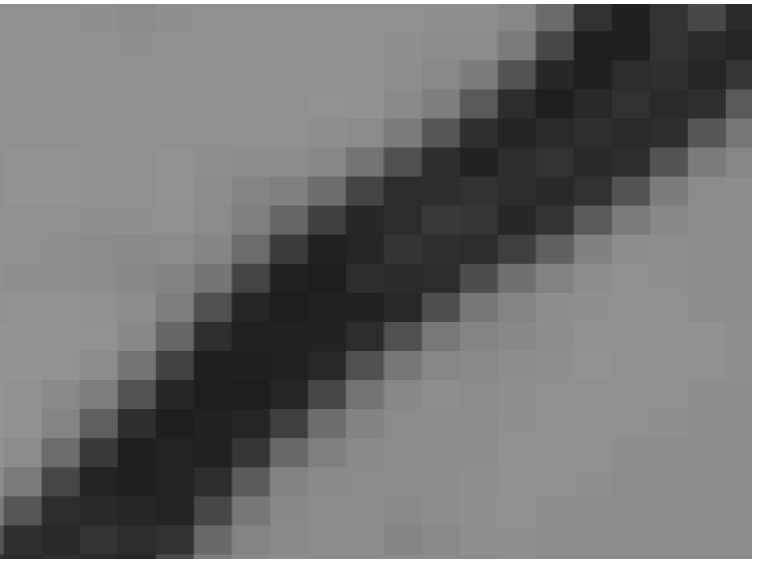
Raw images → Register image sequence → Mapping roots apparition time → **Region adjacency graph building** → Min cost global tracking on the graph

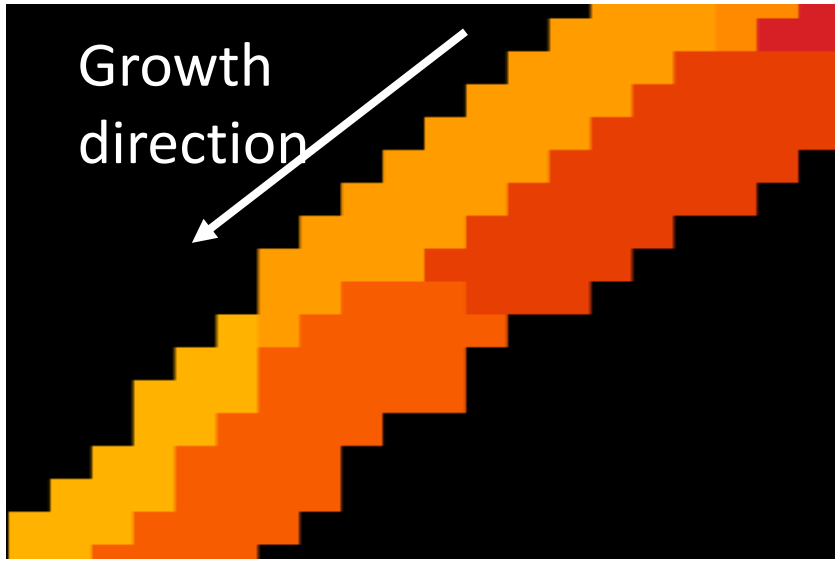




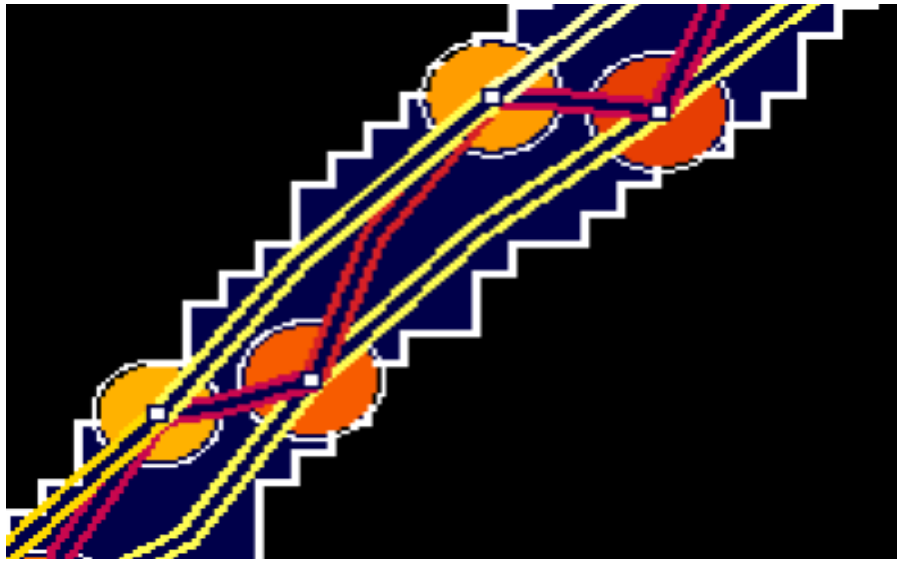
Topological tracking pipeline

Raw images → Register image sequence → Mapping roots apparition time → **Region adjacency graph building** → Min cost global tracking on the graph



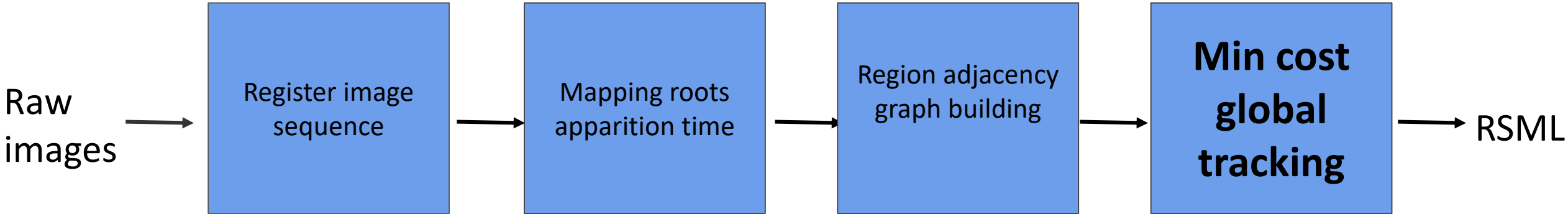


Date map

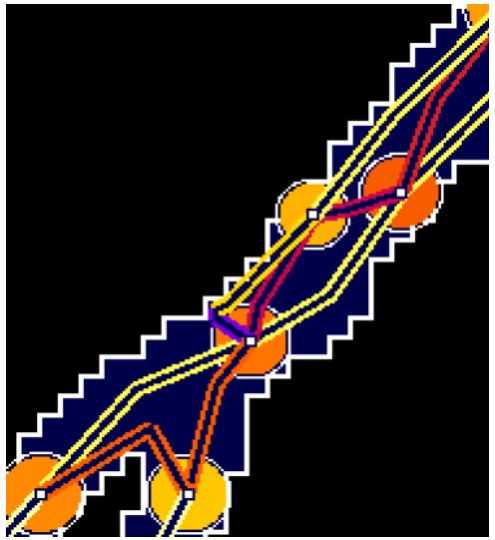


Region Adjacency Graph

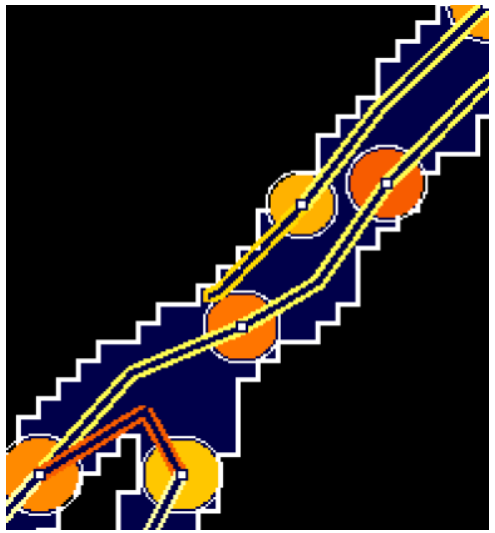
Topological tracking pipeline



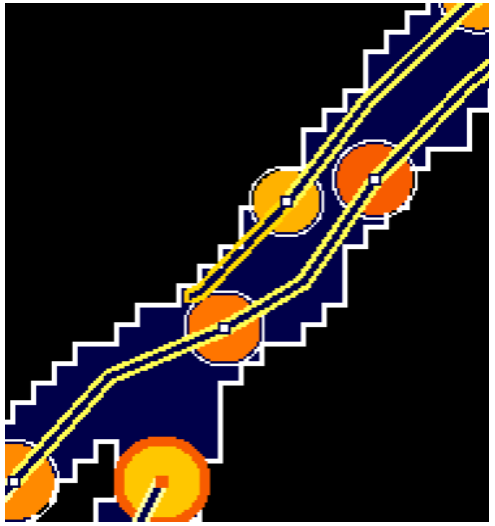
The situation



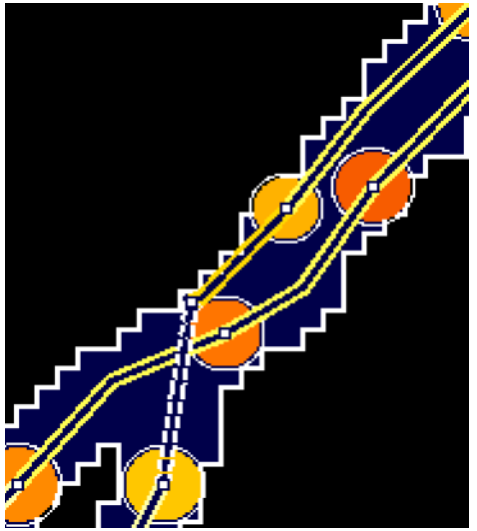
0-Initial graph



1-Minimum directed spanning tree (Edmonds)

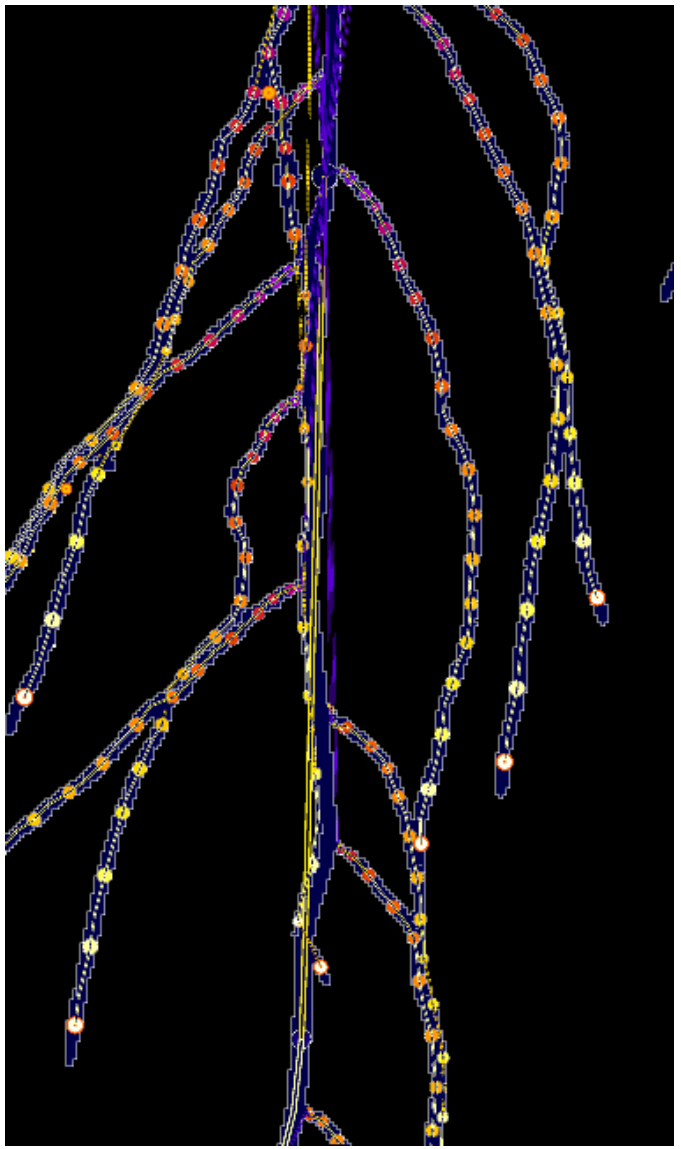


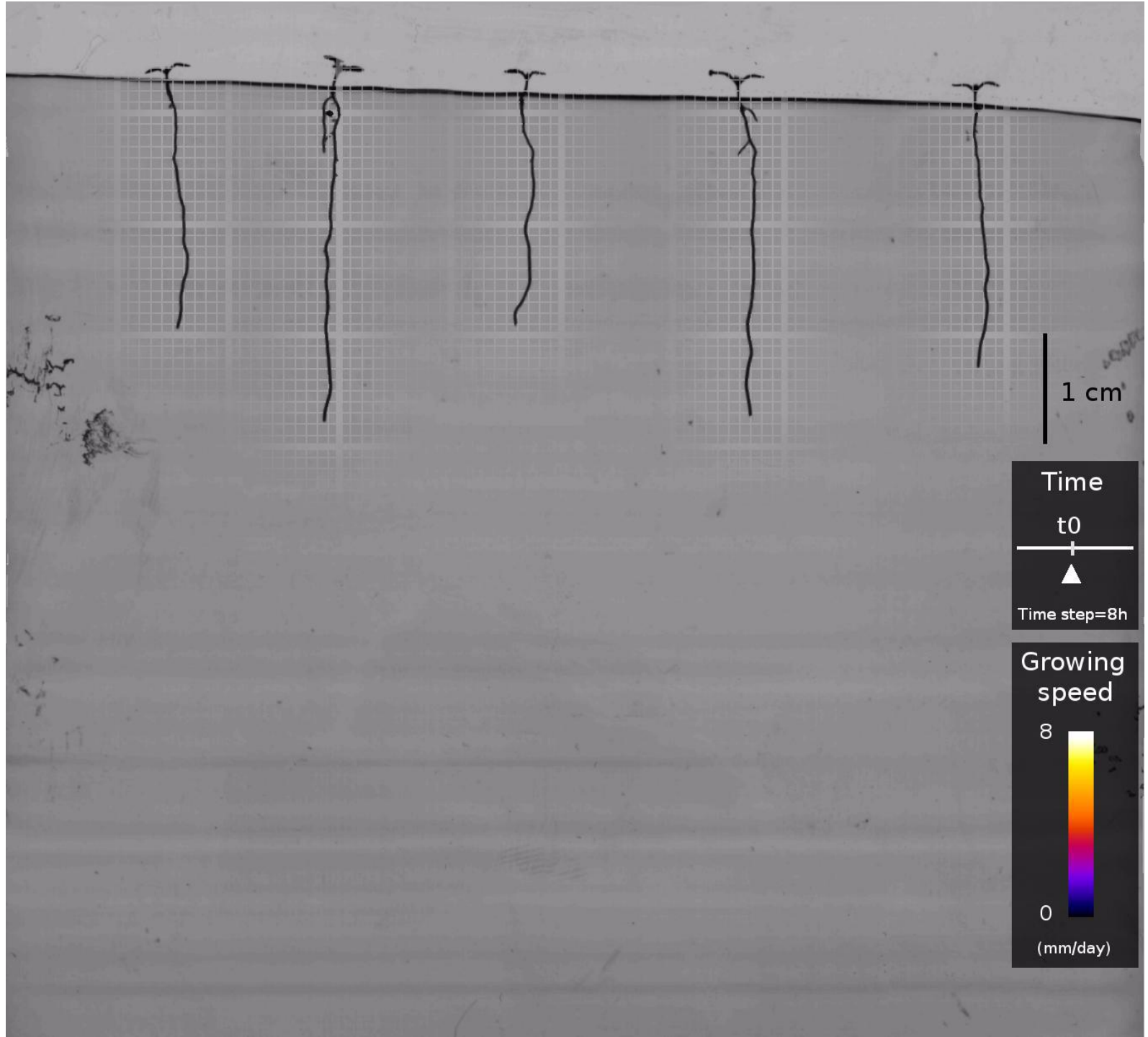
2-Keep only best successor



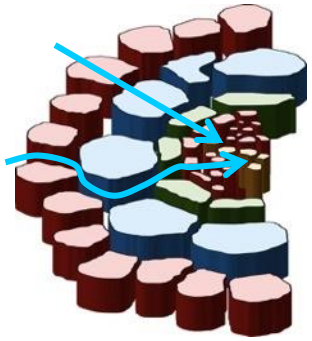
3-Min cost reconnection (Hungarian algorithm)

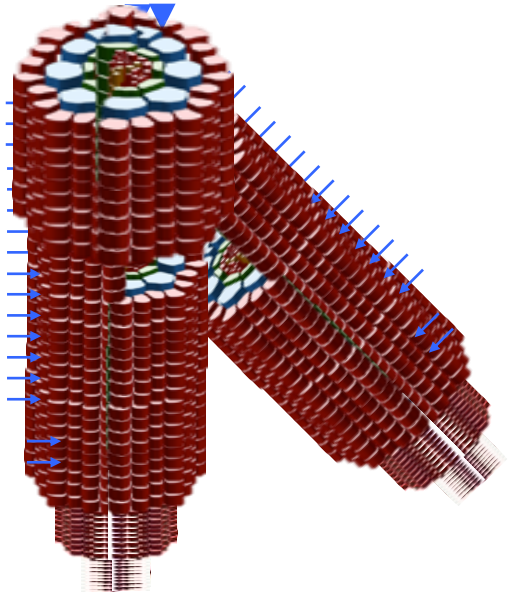
Results on complex data

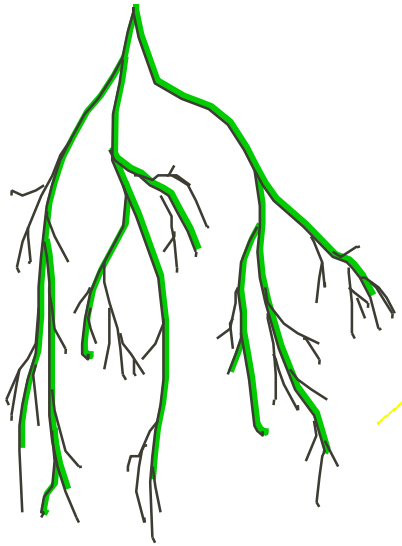


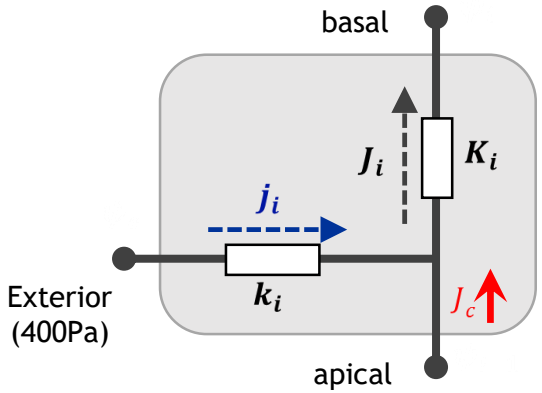

1 cm
Time
t0
Time step=8h
Growing speed
8
0
(mm/day)

Root Hydraulic Architecture: HydroRoot model







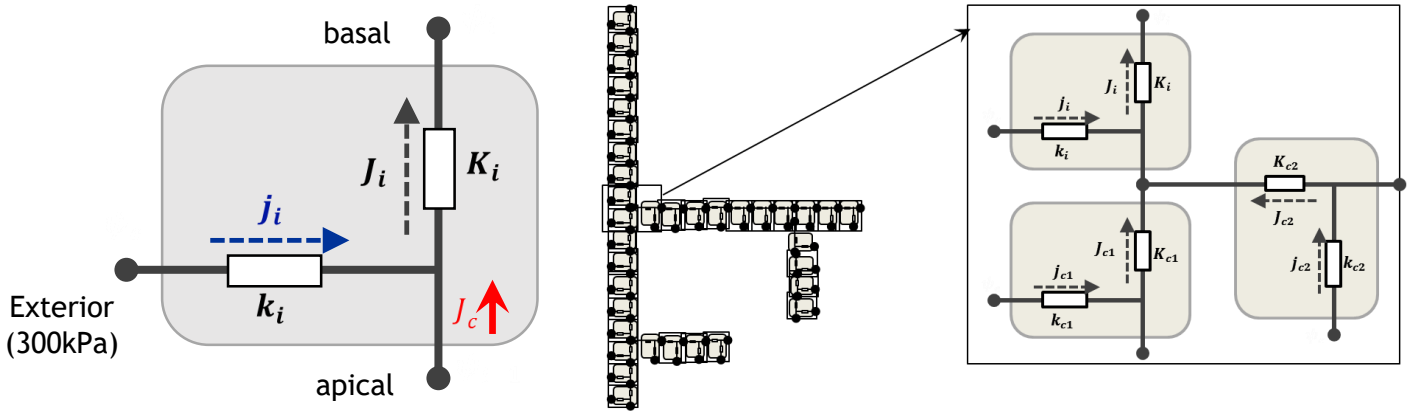


From a hydraulic unit to the whole root water transport (arabidopsis)
Boursiac, Pradal, et al., Plant Physiology, 2022
https://github.com/openalea/hydroroot

Hydroroot Model: electrical analogy

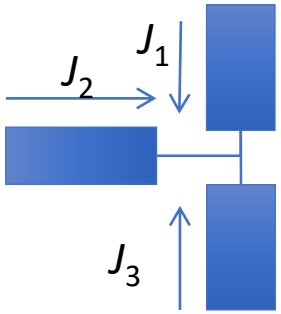
The root system is a MTG ..

….on which we add water flows



D'arcy law $J = K \Delta\Psi$

Millman's law: $\Sigma J_i = 0$



Important hypotheses of our model:

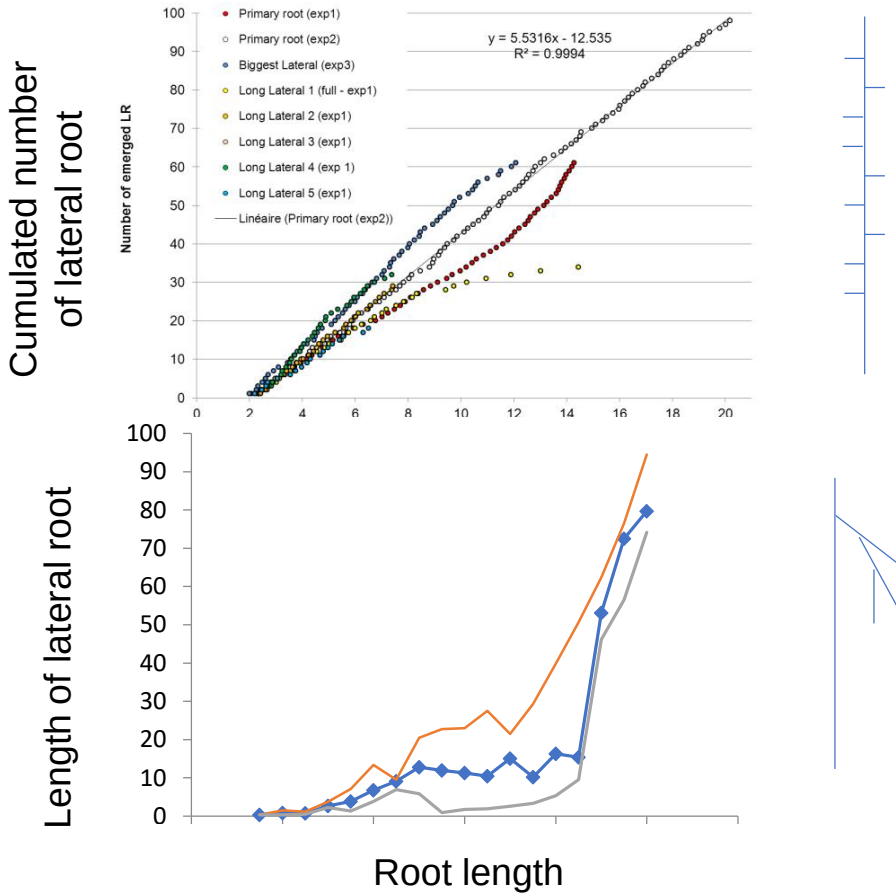
- The diameter of the root is constant
- The radial hydraulic conductivity is constant
- Isotropic external water potential

Explicit linear solver using MTG Traversal

OpenAlea

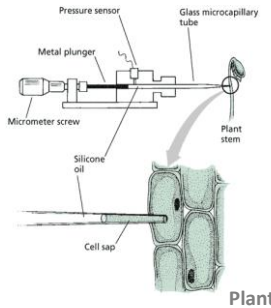
Model parametrisation: phenotyping vs simulation

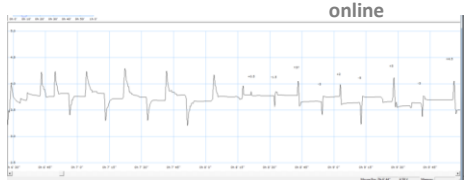
Architecture: building up a root



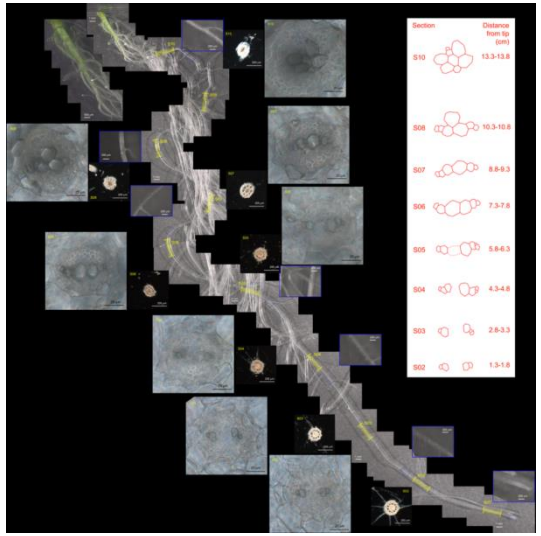
Conductivities: adding water flow

The cell pressure probe

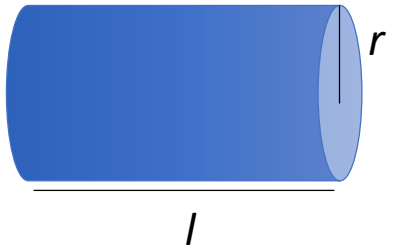




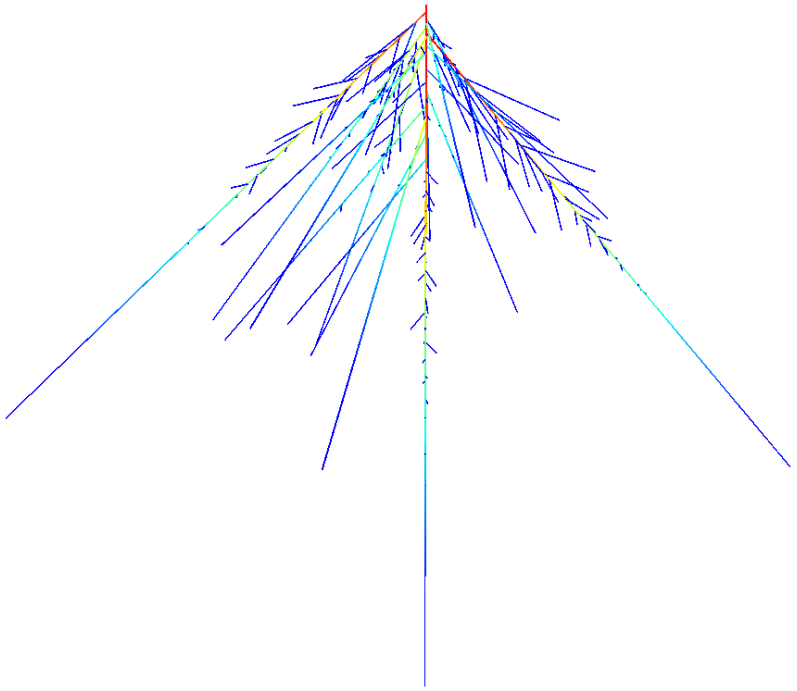
Poiseuille's law



$$R = \frac{8hl}{\rho r^4}$$



Reverse engineering of hydraulic architecture



Model inversion on 12 individuals:

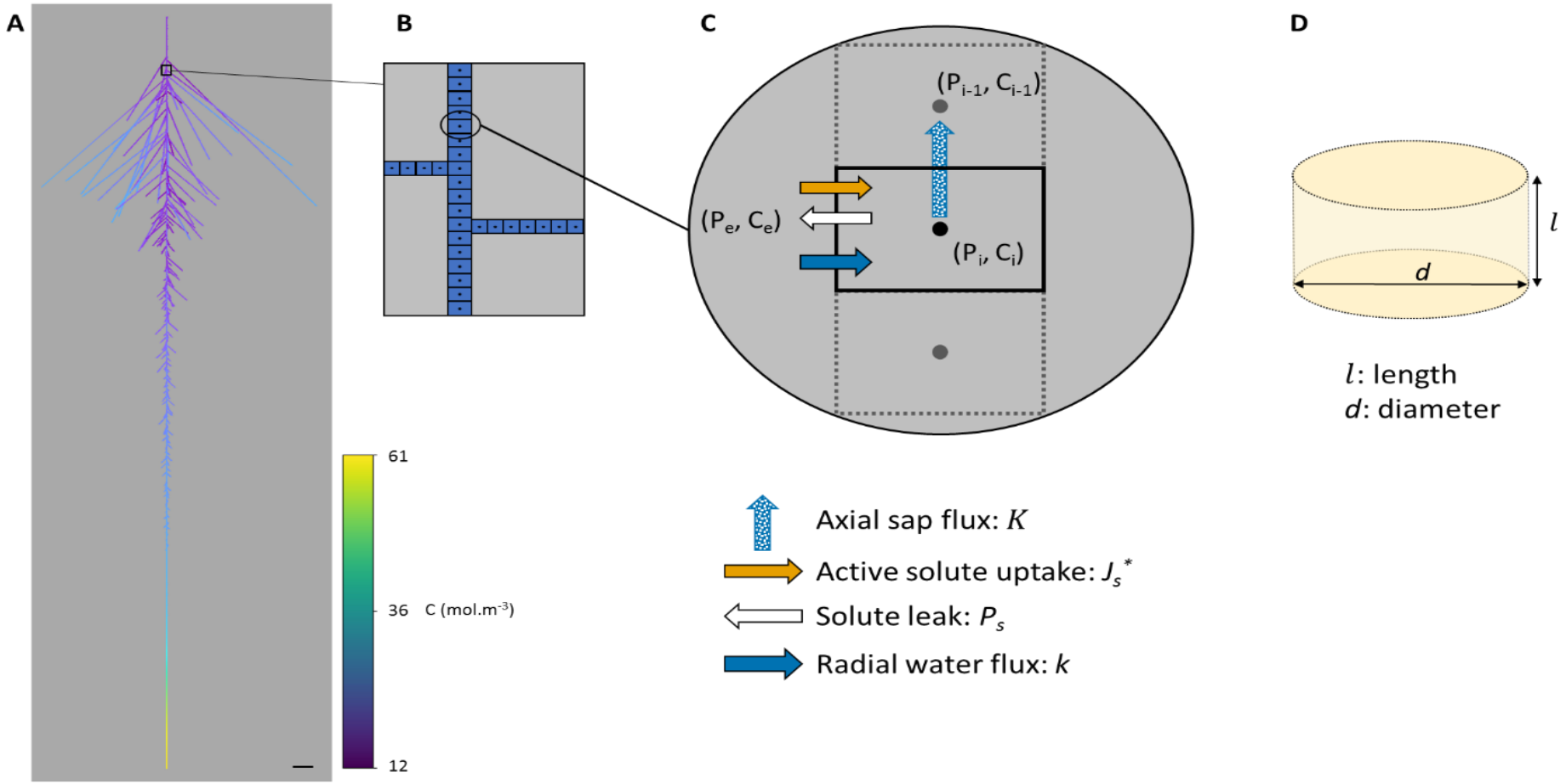
32-154 $m.h^{-1}.Mpa^{-1}$

92,5 average

Estimating radial conductivity by model inversion in hydropony on wild type and mutant

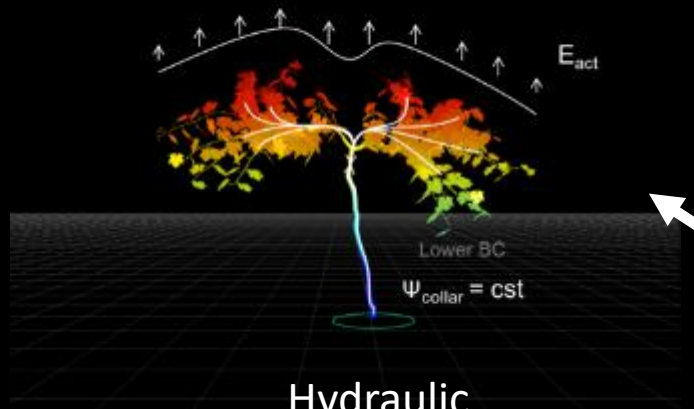
Boursiac, Pradal, et al., Plant Physiology, 2022

Extending Hydroroot: Modelling active and solute transport

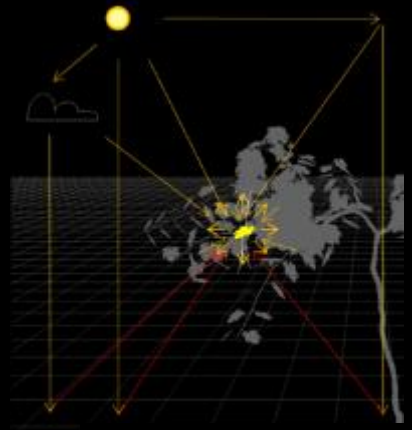


Bauget et al., JXB, in rev.

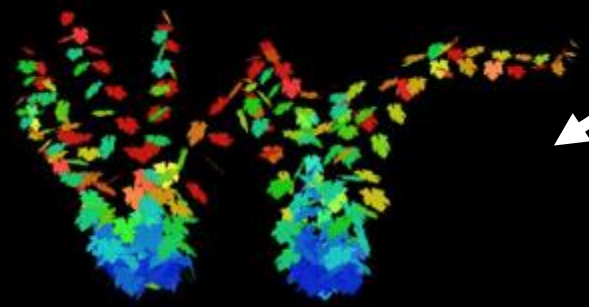
Modelling Shoot Hydraulic Architecture



Hydraulic



Energy budget

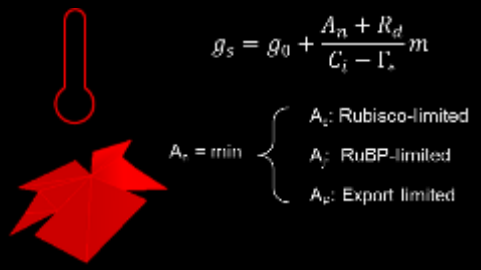


Light interception

Central Data Structure (MTG)

Grapevine

HydroShoot model

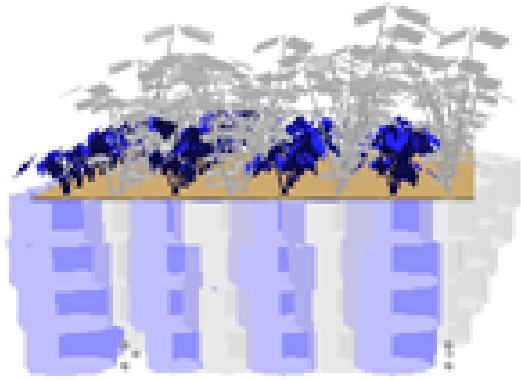


Gas exchange

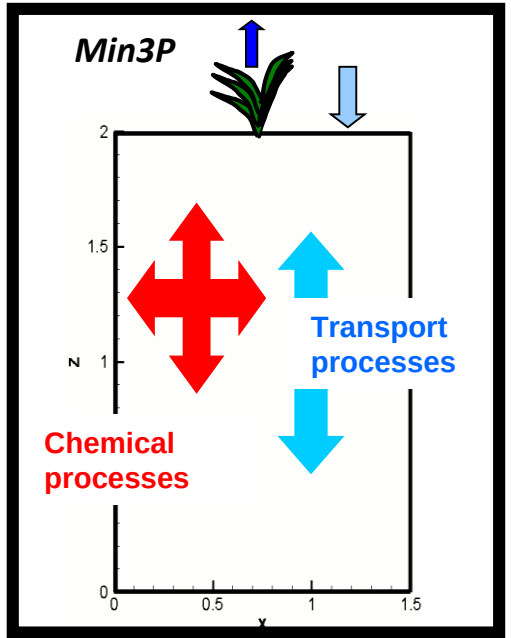
Hydroshoot: Albasha et al., 2019, in silico Plants

Coupling Shoot / Root / Soil in Crop Mixtures

- Modelling Shoot-Shoot competition for light
- Modelling Root-Root competition for water/nutrient uptake
- Modelling Soil processes
  - Min3P: Gerard et al., 2008
  - STICS soil model : Brisson et al., 2006
- Simulating all together (Braghiere et al., 2020)



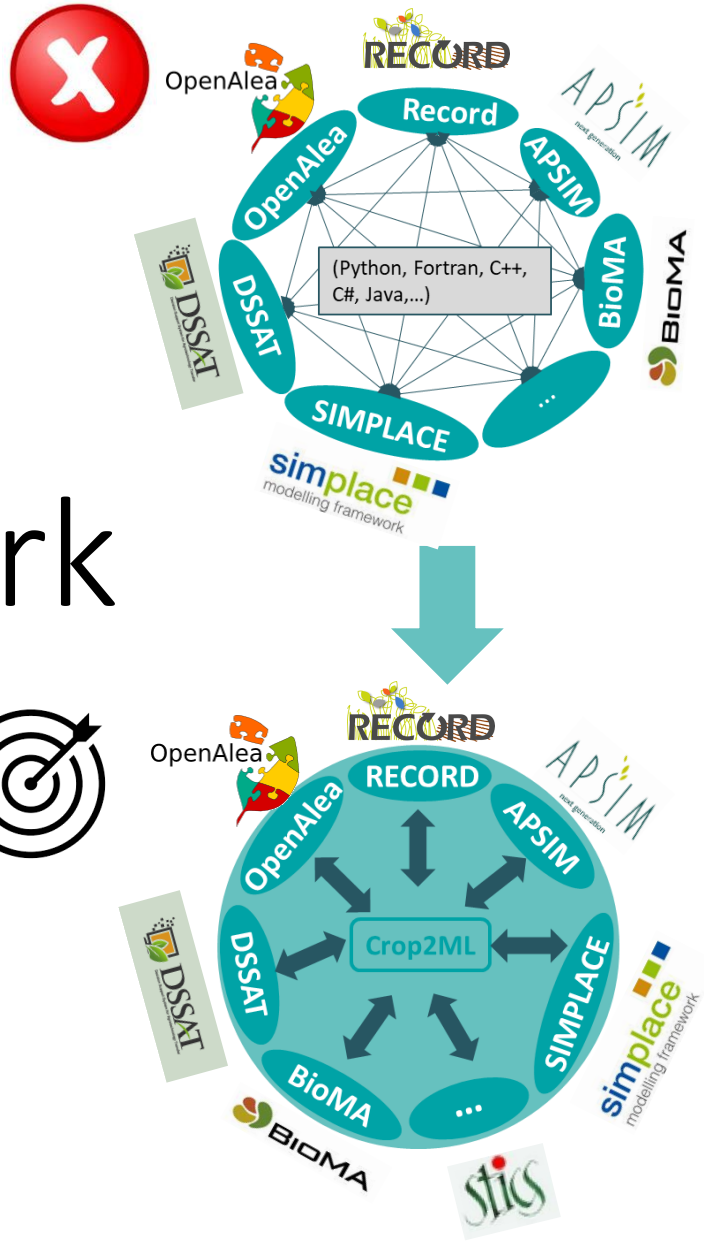
Louarn et al., 2014



Gerard *et al.*, 2008

Crop modelling framework interoperability

Crop2ML: https://crop2ml.org/

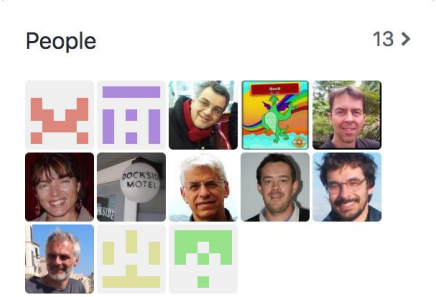


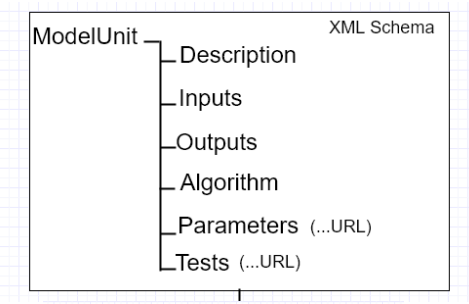
Crop2ML : Toward a common crop modelling language

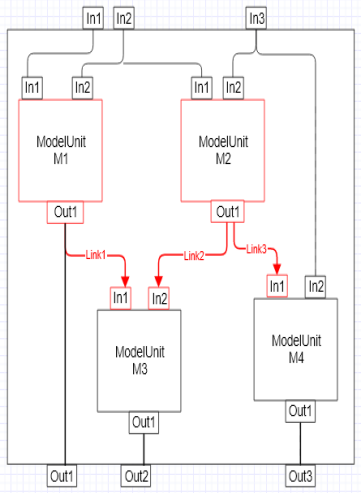
AgMIP The Agricultural Model Intercomparison and Improvement Project

The Agricultural Model Echange Intiative (AMEI)

STICS APSIM INITIATIVE DSSAT RECORD OpenAlea simplace modelling framework BioMA







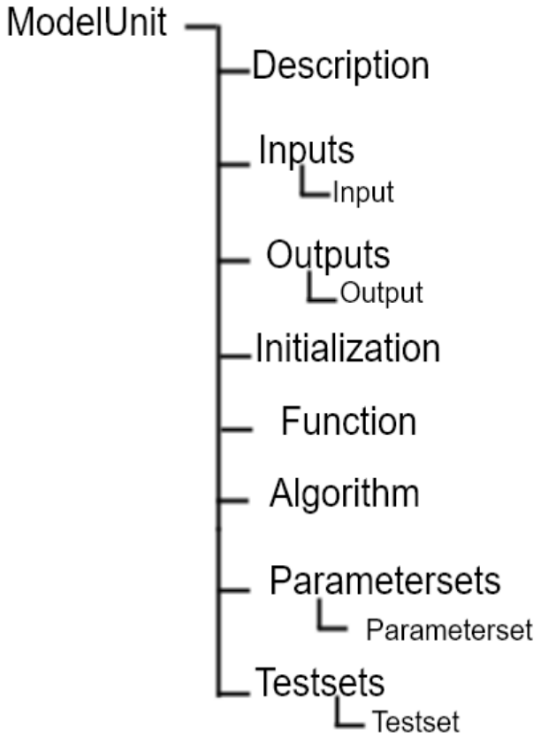
Crop2ML

- Semantic and modular representation of crops models using a **common language**
  - **a subset of Python (Cython)**
- Model Unit with Algorithm in different languages
- Model Composition
- Automatic Import/Export to different platforms

https://github.com/AgriculturalModelExchangeInitiative/

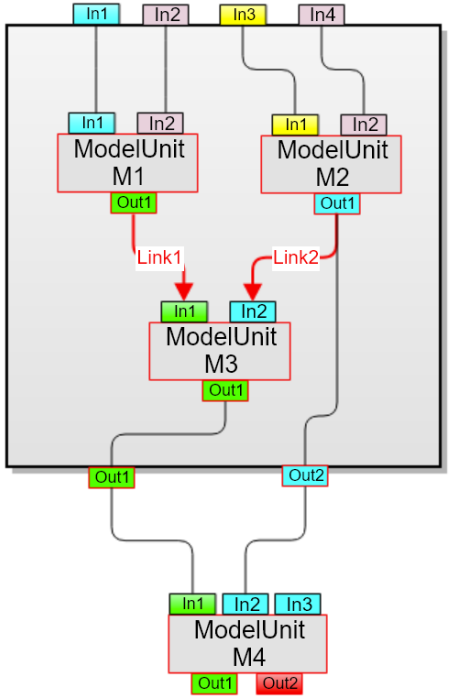
Generic Model representation in Crop2ML with CyML

- Model specification: Framework independent conceptual model (XML-based description)
- Model algorithm: Formal rules to describe ecophysiological processes (Algorithms) or functions



ModelUnit

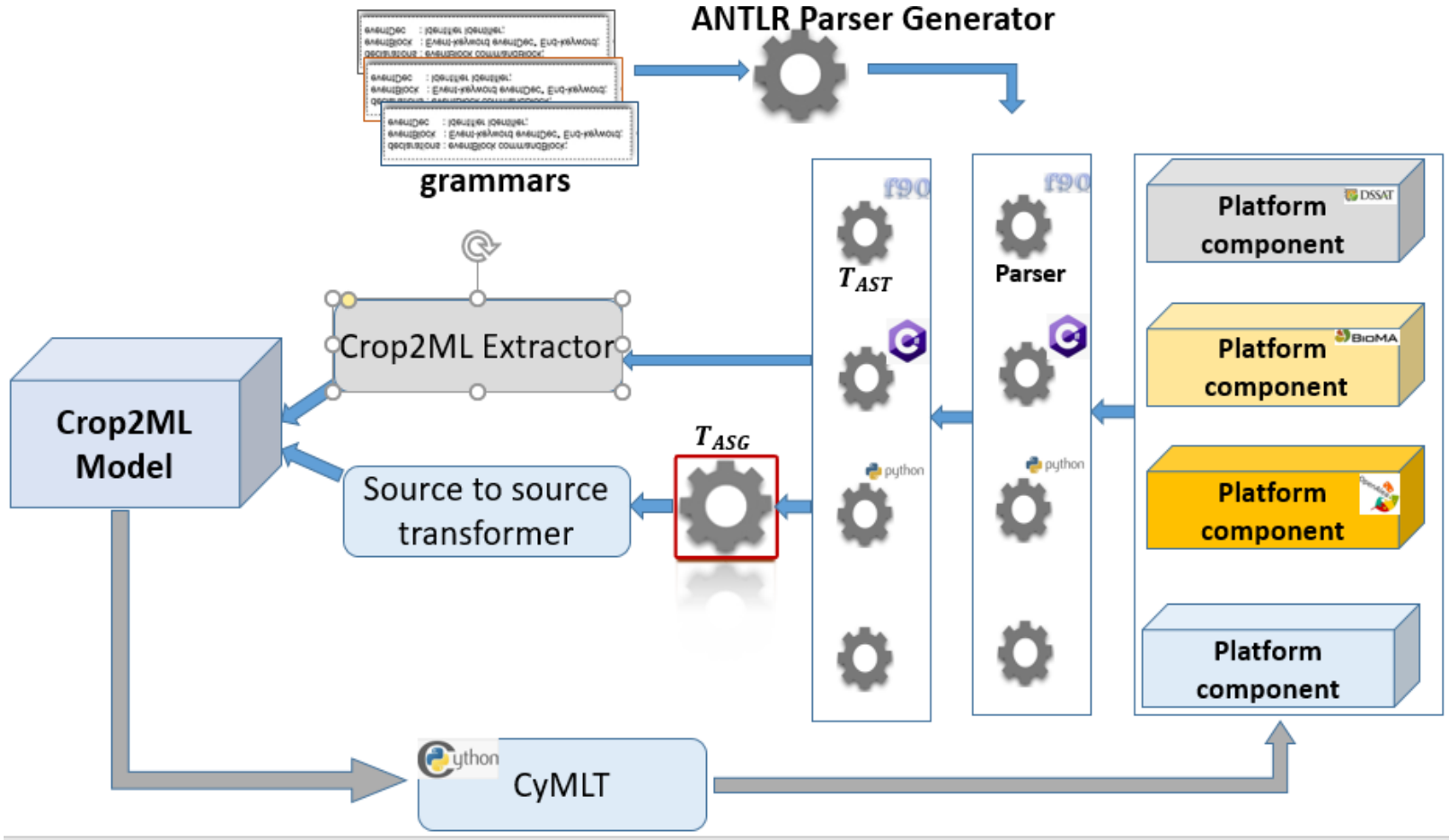
Composition



ModelComposite

Midingoyi et al., 2021, Env. Mod. & Soft.

Crop2ML : Model to model transformation



Midingoyi et al., 2020, *in silico plants*
Midingoyi et al., 2022, *in prep.*

Automatic Model transformation

Soil temperature

simplace modelling framework

BioMA

stics

DSSAT Decision Support System for Agrotechnology Transfer

OpenAlea — Python

BioMA — C#

DSSAT Decision Support System for Agrotechnology Transfer — Fortran

stics — Fortran

RECORD — C++

Other and Non specific platform

Take Home Message

- OpenAlea is an open source modelling community
- 3D Architecture & development can be capture by Phenotyping methods
- Functional Models can process either simulated or reconstructed architecture (in-silico experiments)
- There are connexions between plant and crop modelling communities
- Software reuse is key inside platforms (OpenAlea), but also between platforms (Crop2ML)

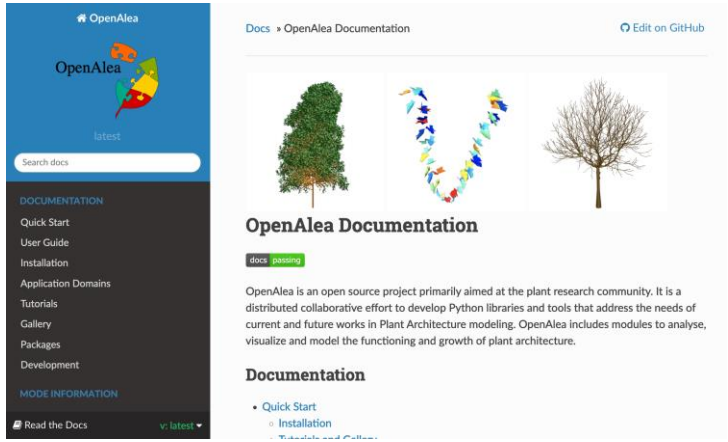
Research Challenges

1. **Automatic field** phenotyping
2. **Semantic** composition of FSPM and crop models
3. Deep Learning
    1. **Automatic training** with 3D+t annotated synthetic data (topology/geometry)
    2. **Physically-informed Neural Networks** with process-based models
    3. **Upscaling** mechanistic models with meta-models

Questions?

CONDA

https://github.com/openalea
https://github.com/openalea-incubator
https://github.com/openalea-training



https://openalea.rtfd.io