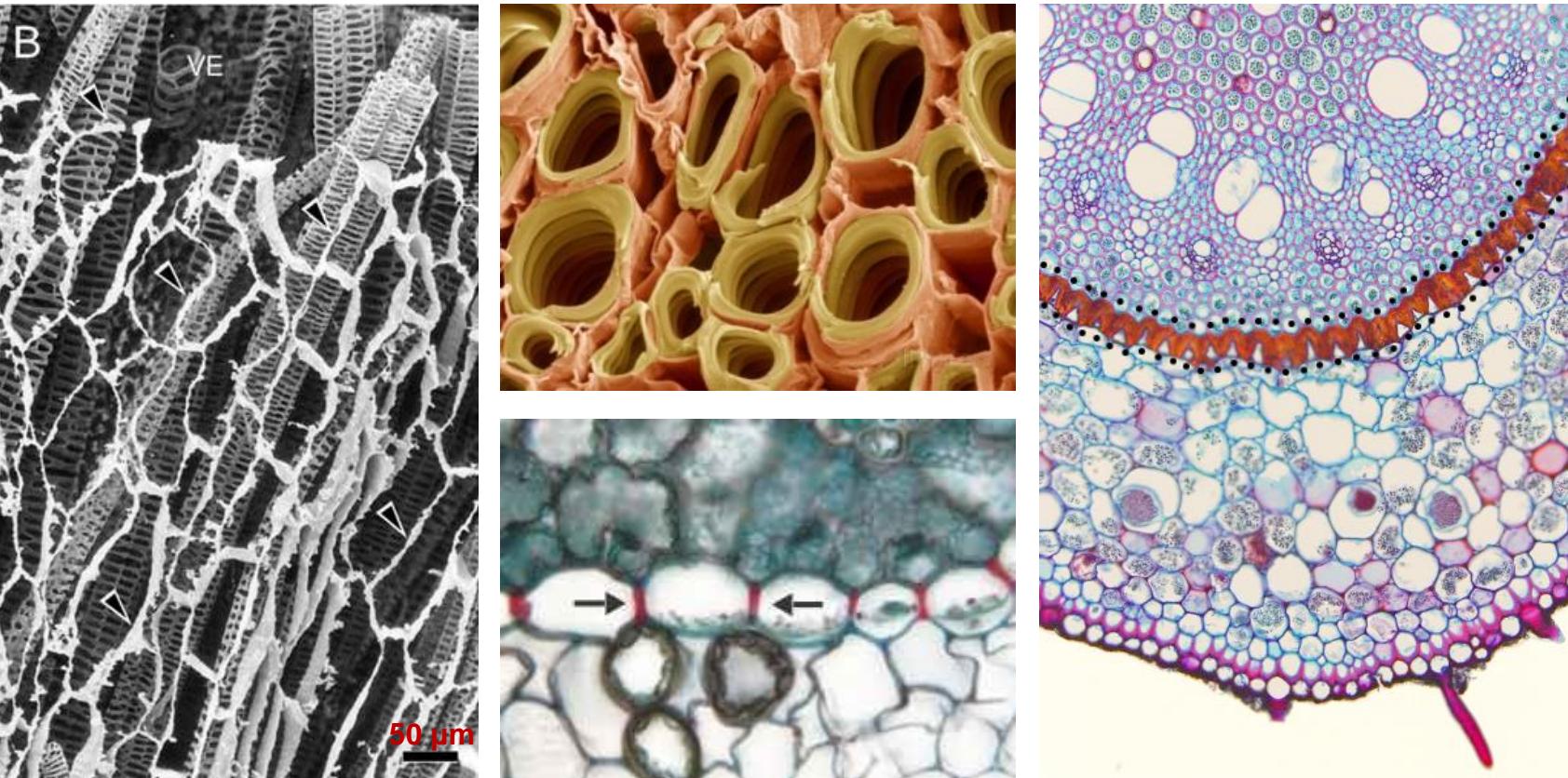


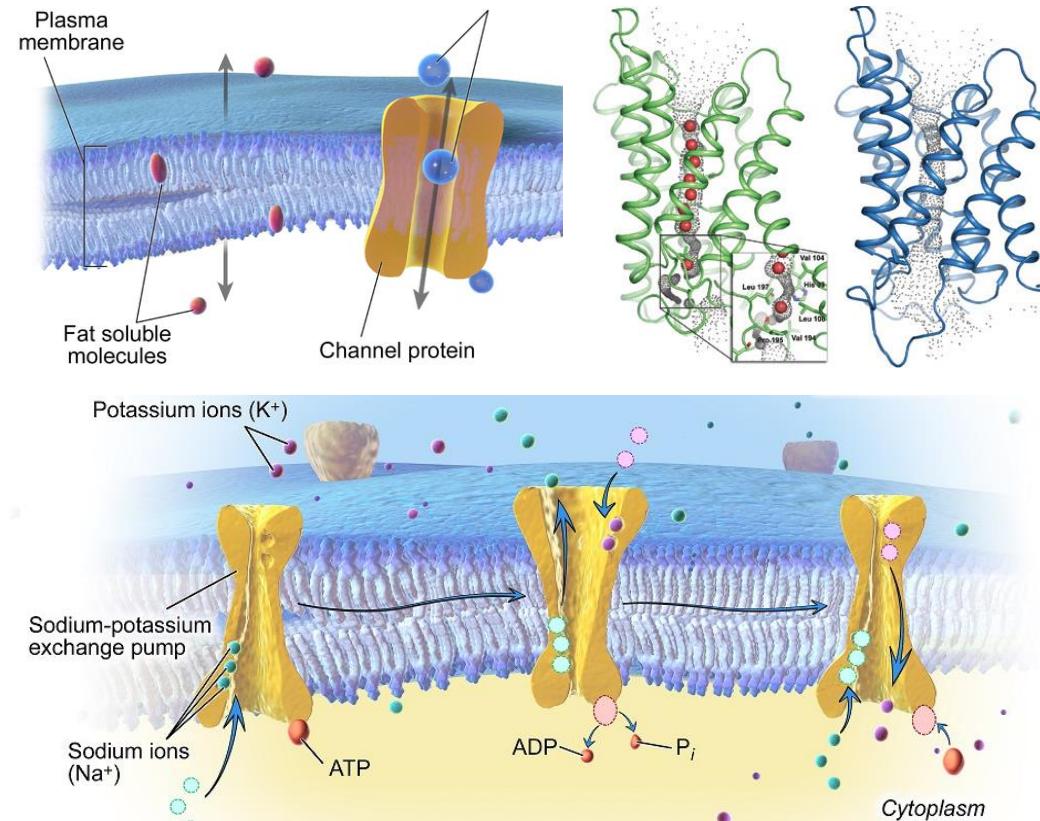
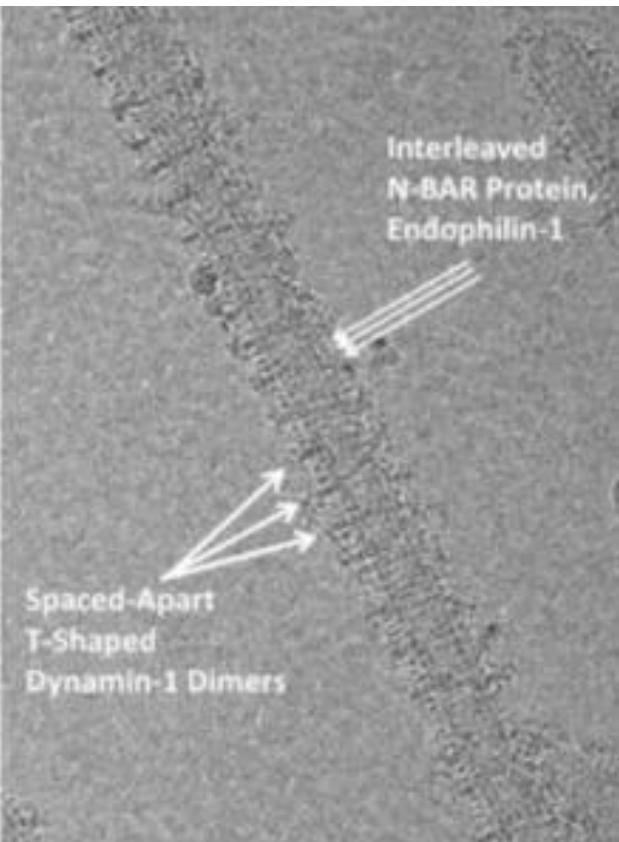
# Apoplastic structures

- Scaffolds: Physical **separation** of compartments
- Thickening: Physical **support** against implosion / explosion
- Pipes: Long distance water **transport**



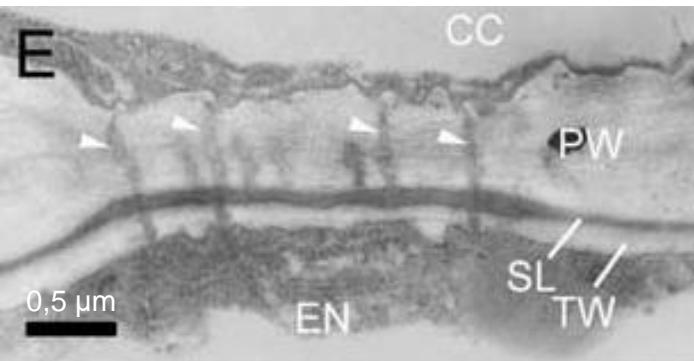
# Transmembrane structures

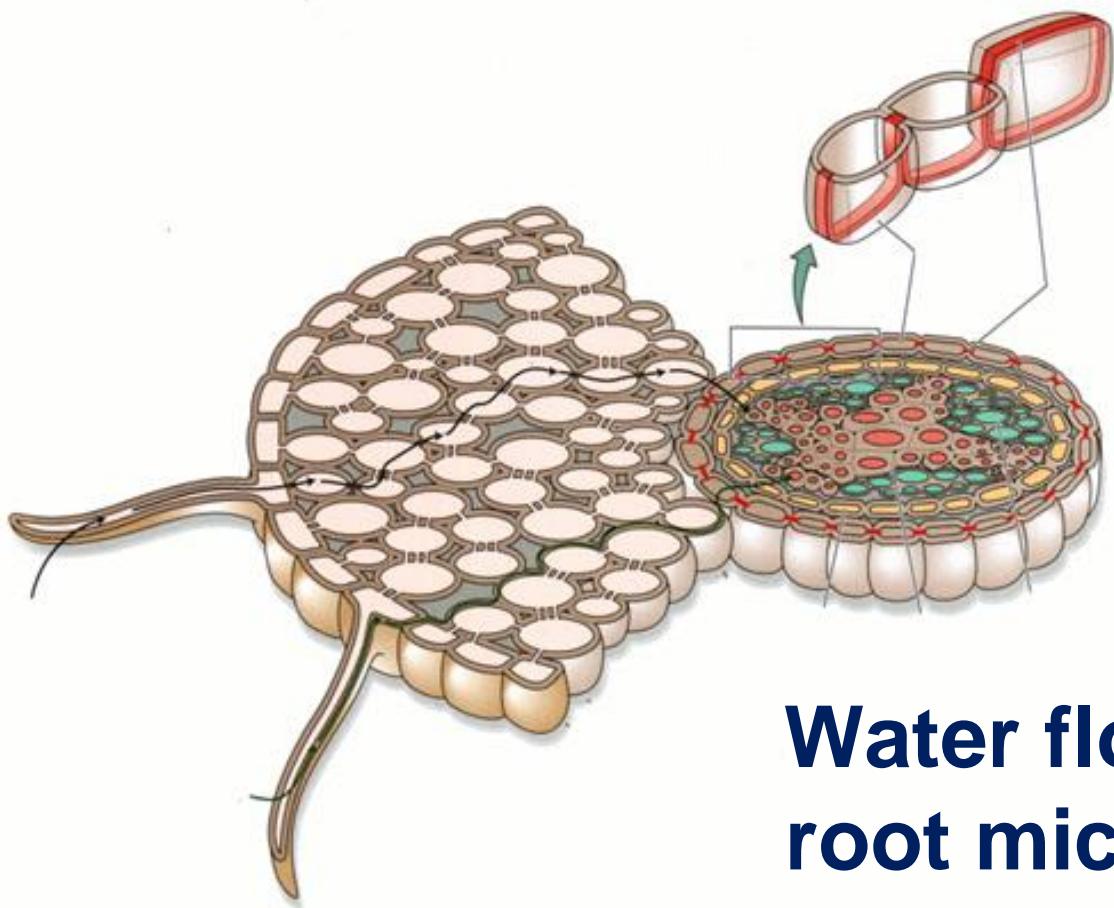
- Pumps: Active **accumulation** of ions / molecules
- Channels: Passive **diffusion** of ions / molecules



# Symplastic structures

- Plasmodesmata: Passive **diffusion** of ions / molecules

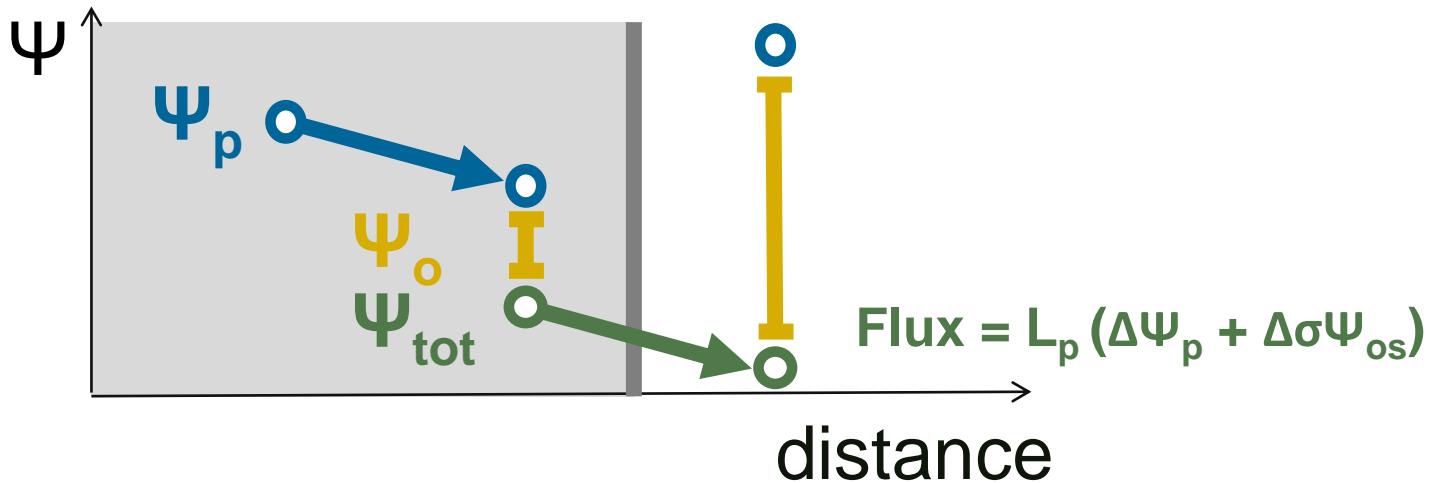




## Water flow across root micro-structures

# Cell level hydrological principles

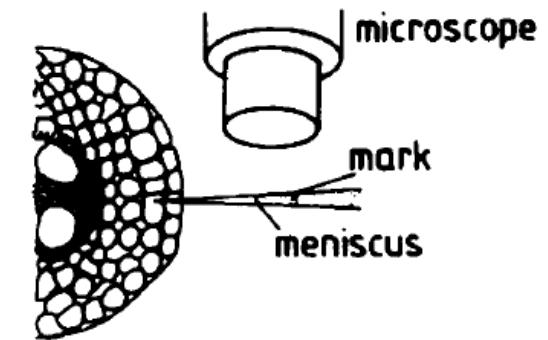
Water flow across  
cell walls & membranes



$$\Psi_{tot} = \Psi_p + \Psi_o$$

where

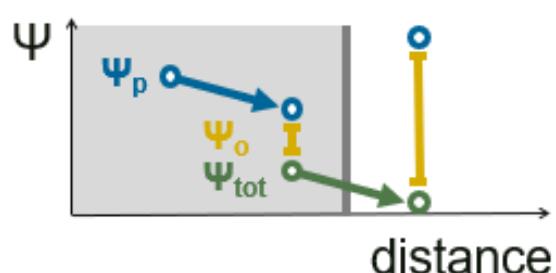
$$\Psi_o = -RT C_{os}$$



Zhu and Steudle (1991)  
Plant Physiol., 95, 305-15

# Current paradigm of water flow across root tissues

Water flow across  
cell walls & membranes

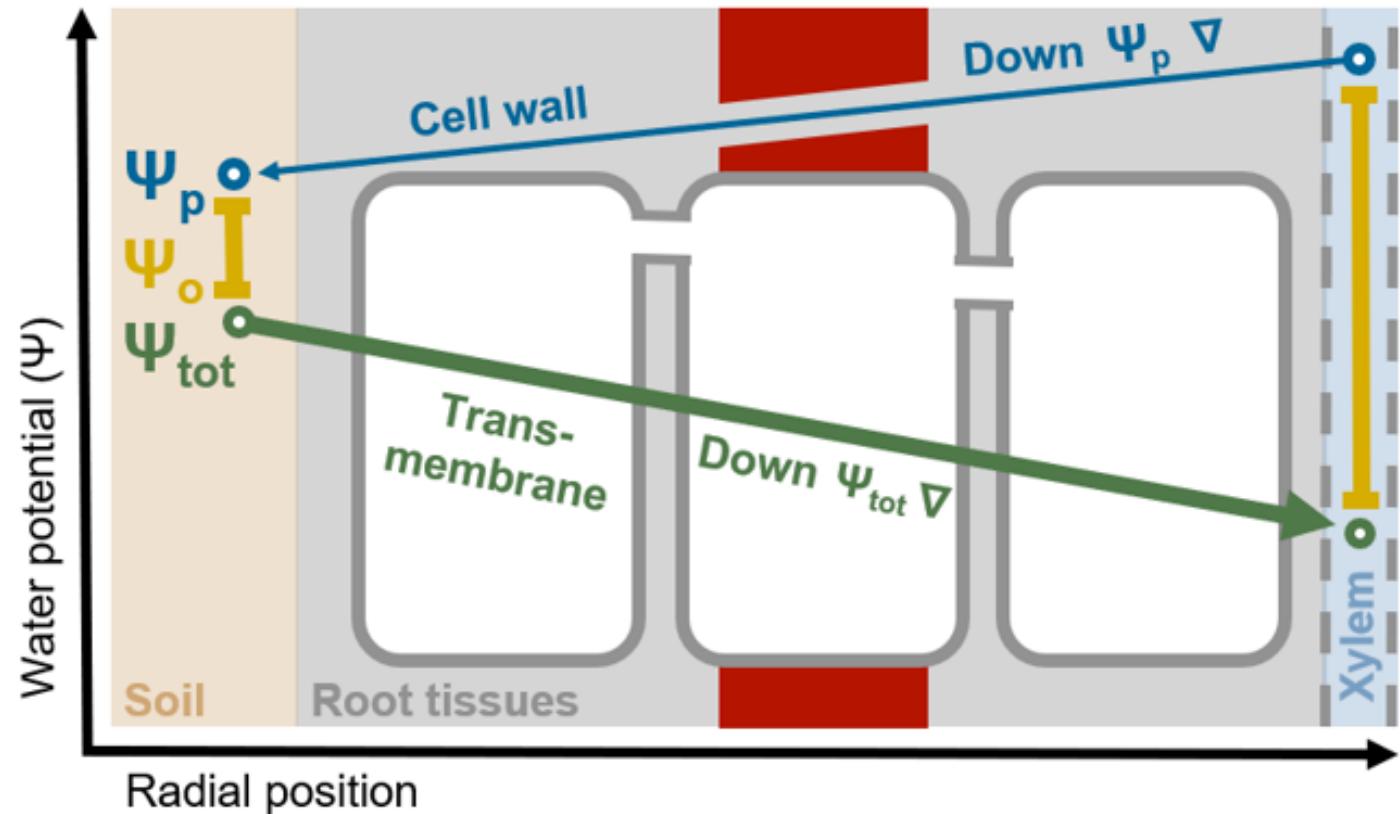


$$\Psi_{tot} = \Psi_p + \Psi_o$$

where

$$\Psi_o = -RT C_{os}$$

Root radial flow is analog to flow across a “big membrane”

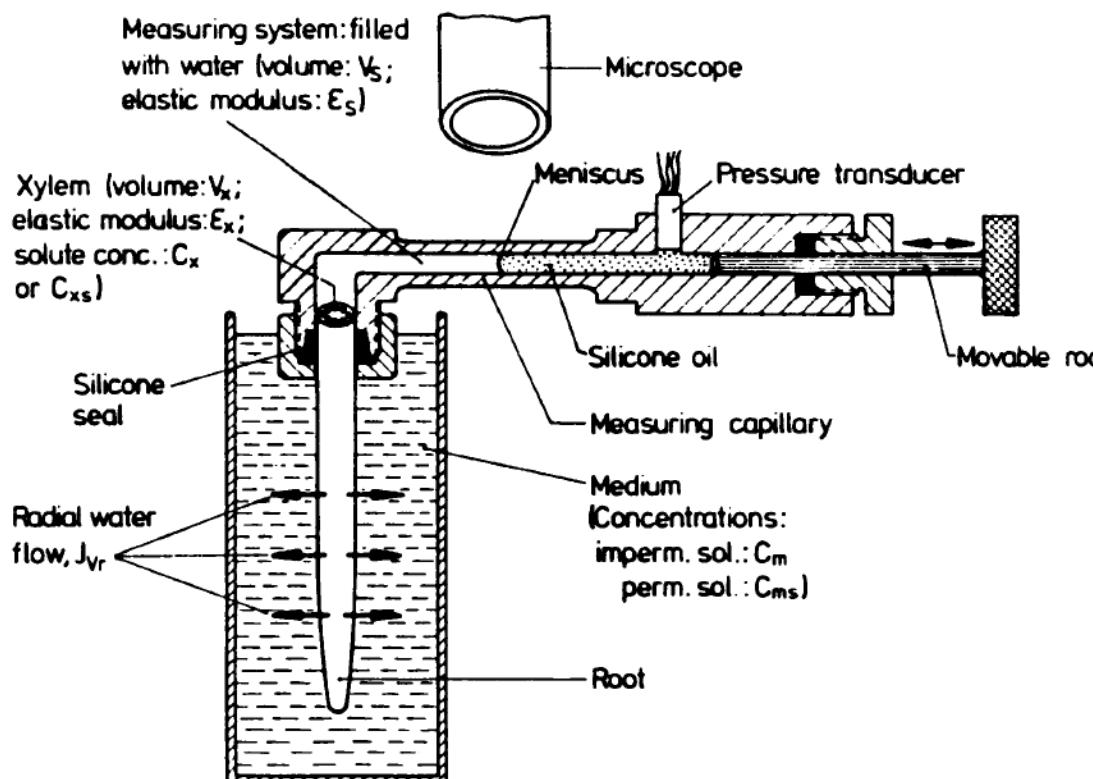


# Root level hydrological principles

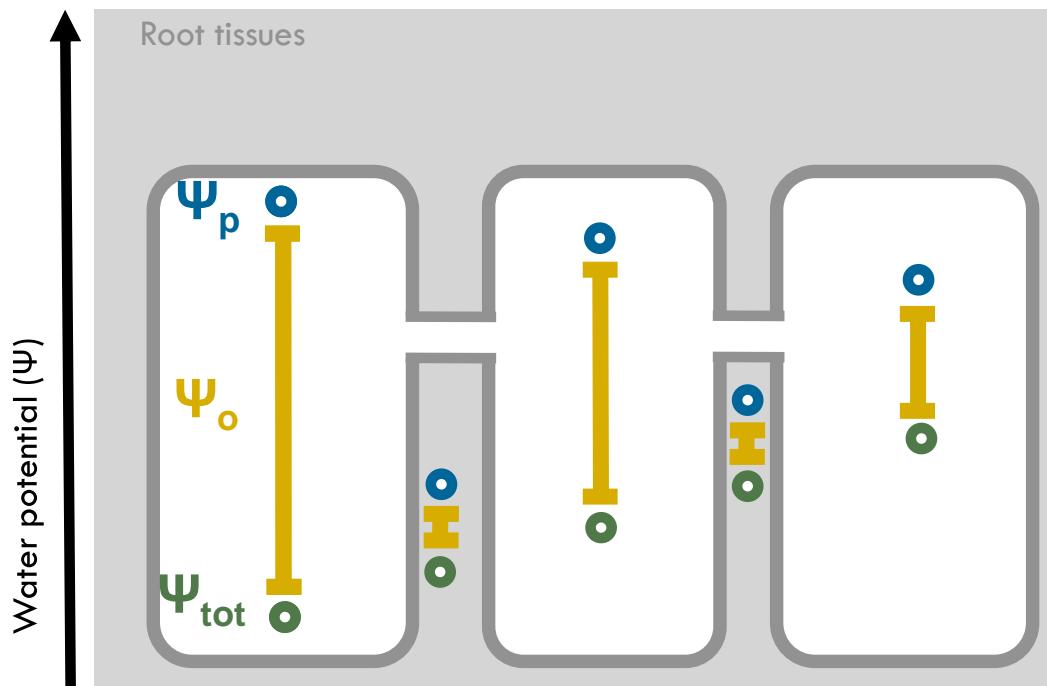
$$\text{Flux} = L_{pr} (\Delta\Psi_p + \Delta\sigma\Psi_o, \text{apo})$$

$$\text{where } \Psi_o = -RT \sum C_o$$

Fiscus and Kramer (1975) PNAS, 72, 3114-8



# Does water flow to the right or to the left ?



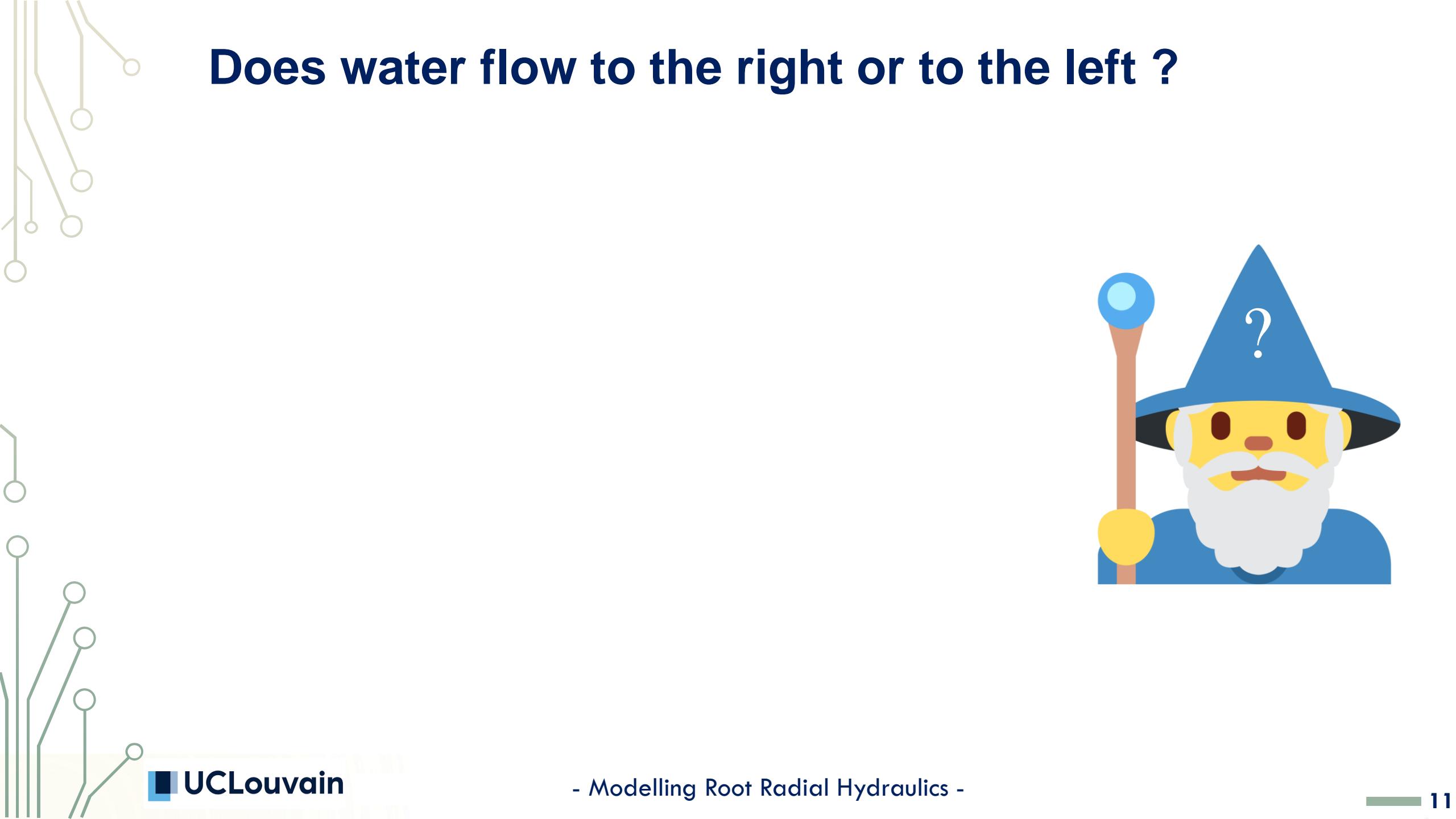
- 1
- 2

Allez sur [wooclap.com](https://wooclap.com)

Entrez le code d'événement dans le bandeau supérieur

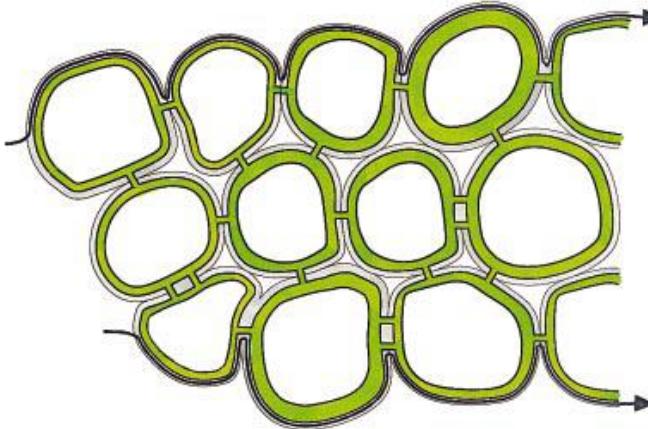
Code d'événement  
**MECHA2219**



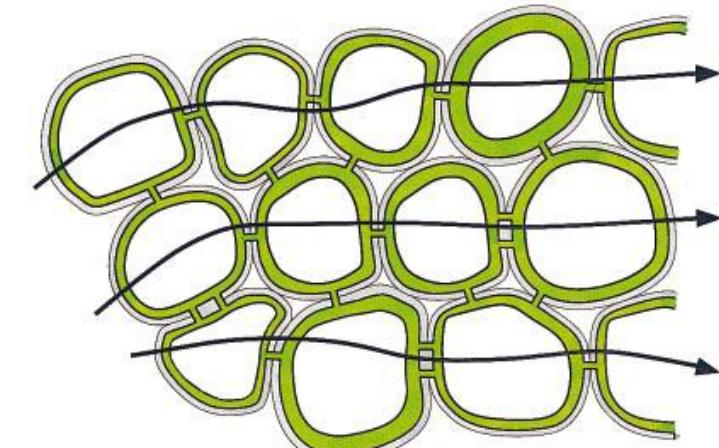
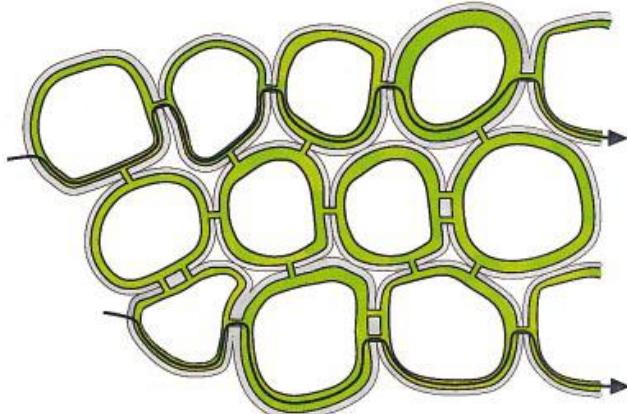


# Does water flow to the right or to the left ?



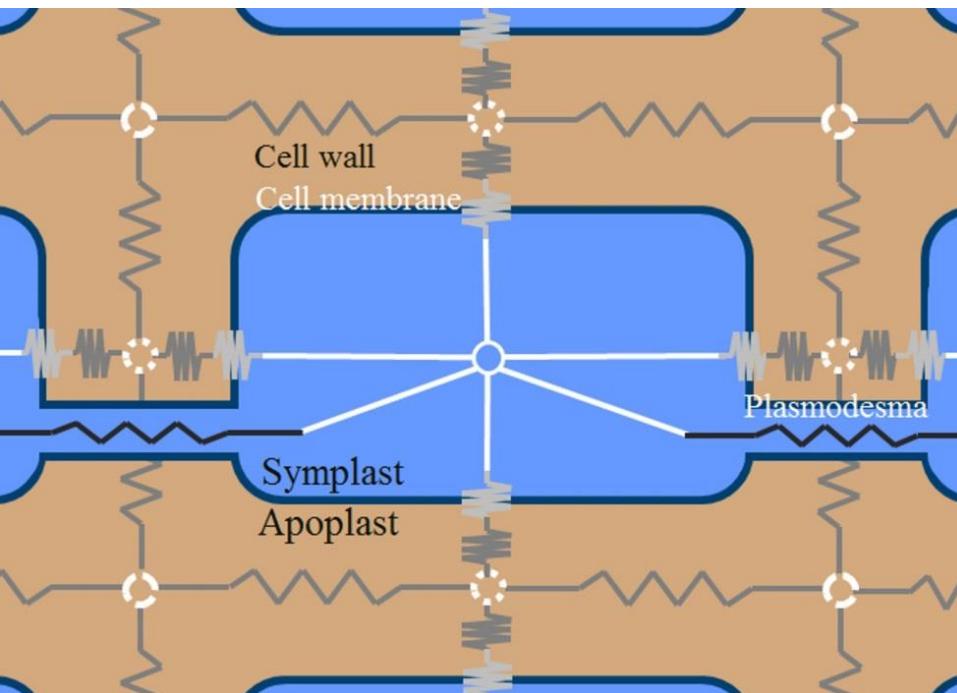


## Setting hydraulic principles on a biological layout



# Cell level hydraulic model

Permeability of cell walls (Steudle and Boyer, 1985), membranes (Elhert et al., 2009), and plasmodesmata (Bret-Hart and Silk, 1994; Warmbrodt, 1985; Clarkson et al., 1987)



Flow principles:

- $\Psi_p$  driven in walls and plasmodesmata
- $\Psi_{tot}$  driven flow across membranes

Plasmod.:  $2.0 \cdot 10^{-4} \text{ cm hPa}^{-1} \text{ d}^{-1}$

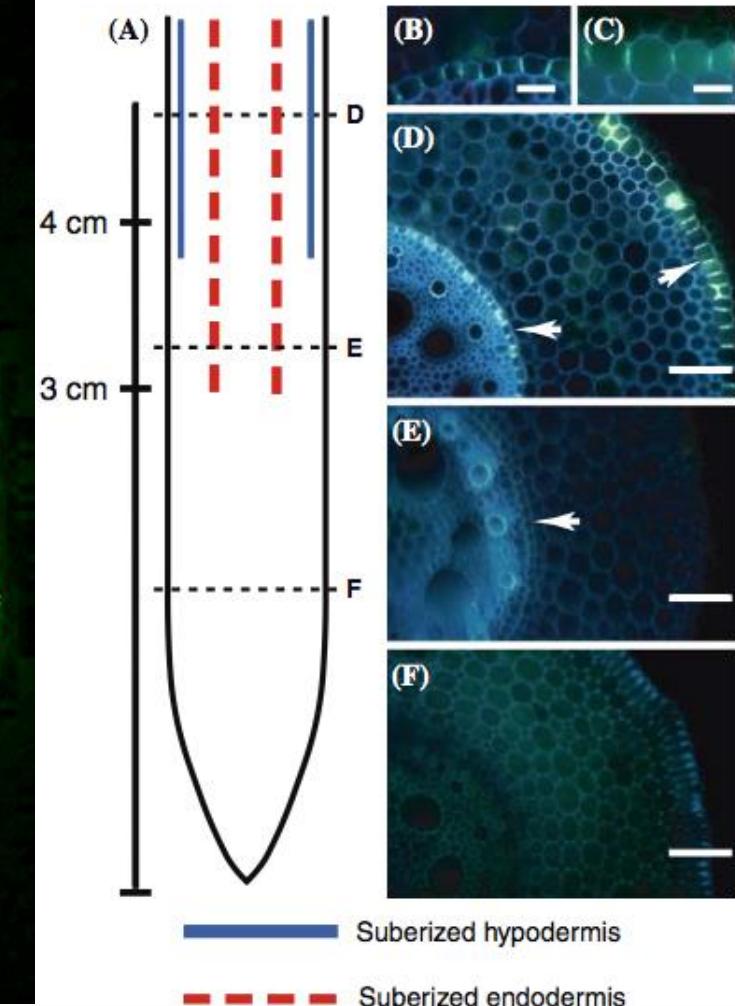
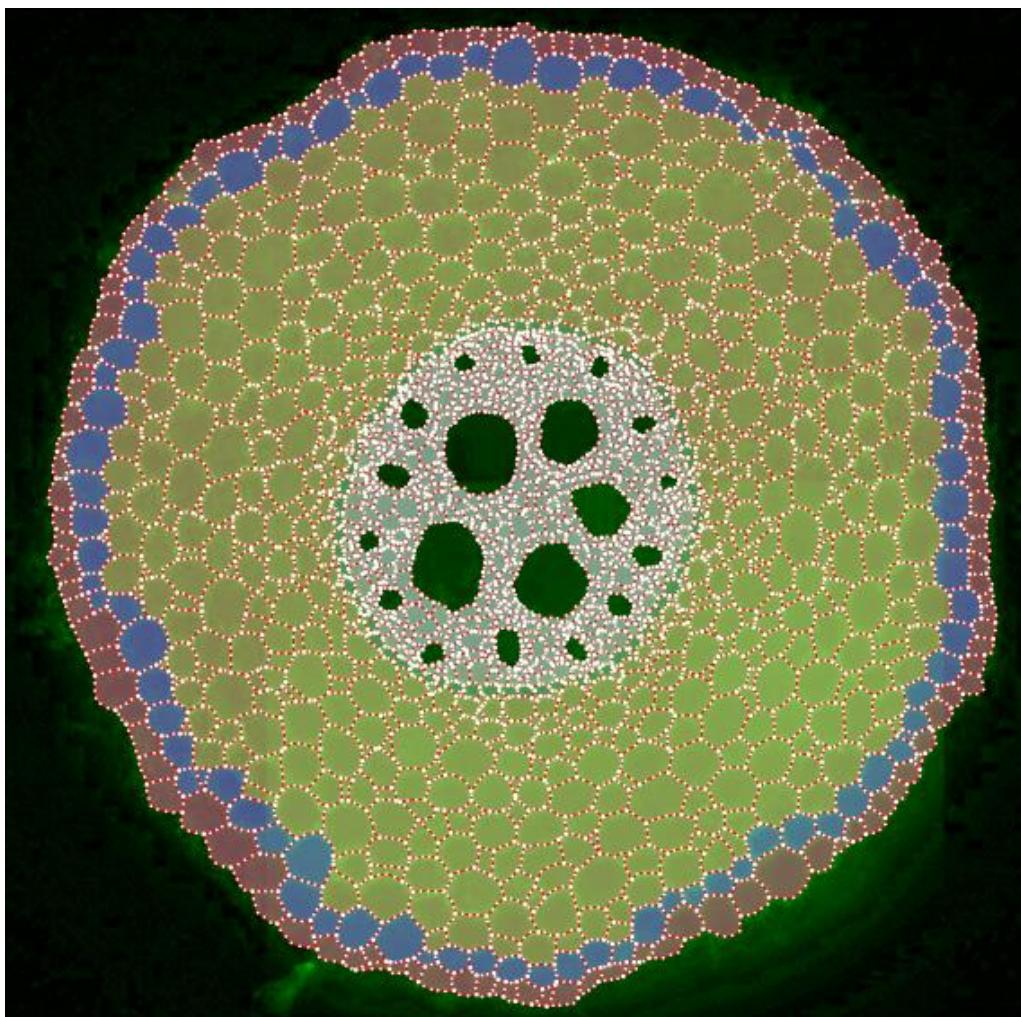
Membrane:  $5.0 \cdot 10^{-4} \text{ cm hPa}^{-1} \text{ d}^{-1}$

Young root:  $1.0 \cdot 10^{-4} \text{ cm hPa}^{-1} \text{ d}^{-1}$

Cell wall:  $0.005 \text{ cm}^2 \text{ hPa}^{-1} \text{ d}^{-1}$

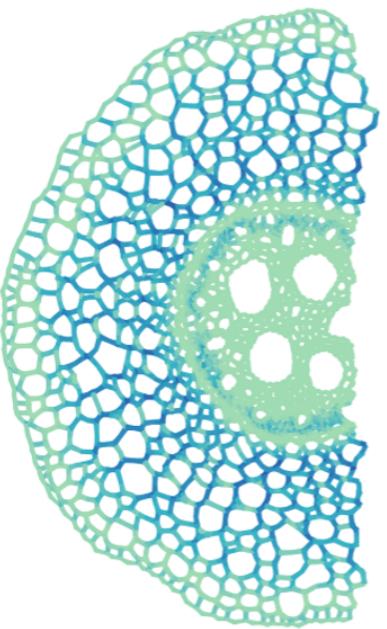
Silty clay:  $0.5 \text{ cm}^2 \text{ hPa}^{-1} \text{ d}^{-1}$

# Root anatomy and location of apoplastic barriers



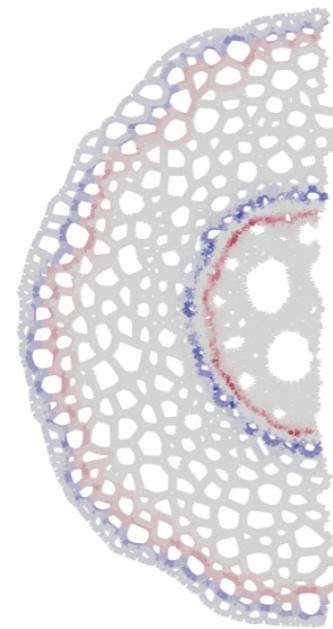
# MODELLING WATER FLOW AT THE ORGAN SCALE

## - MECHA -



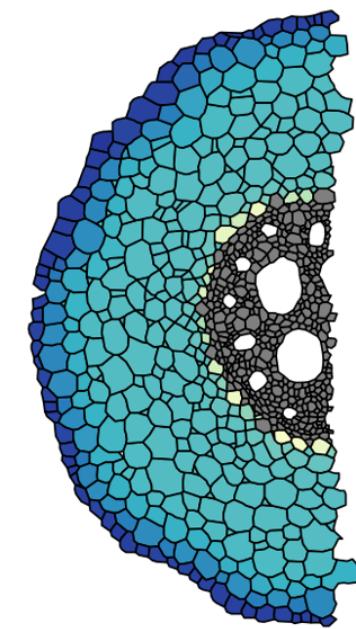
Wall  
fluxes  
 $[1e6 \cdot m/s]$

0.8
0.6
0.4
0.2
0.0



Trans-  
membrane  
flux  
 $[1e7 \cdot m/s]$

2
1
0
-1
-2



Cell  
pressure  
 $[hPa]$

8000
7800
7600
7400



Open Source



[mecharoot.github.io](https://mecharoot.github.io)



Couvreur et al, 2018

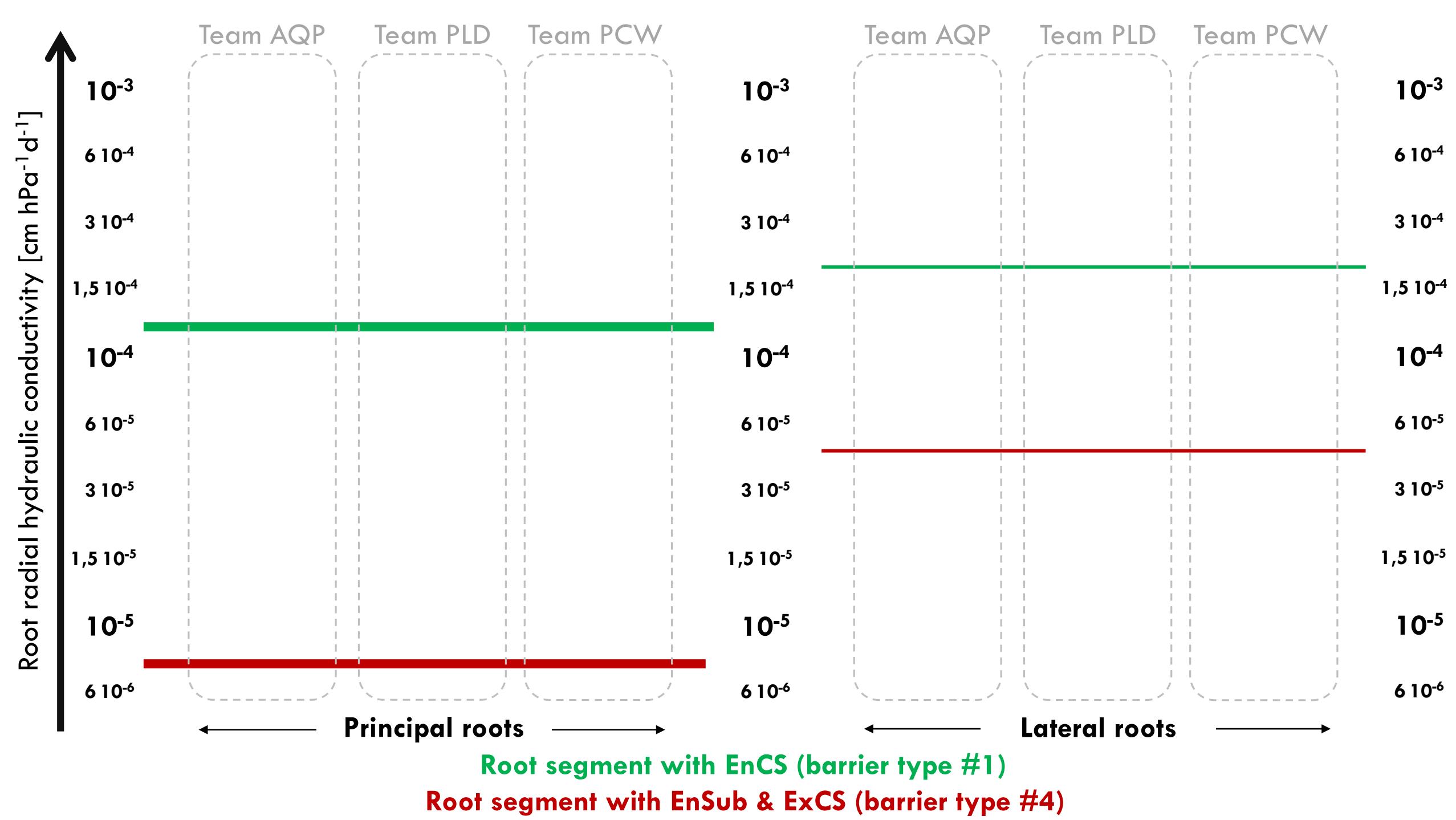
Going with the Flow: Multiscale Insights into the  
Composite Nature of Water Transport in Roots<sup>1[OPEN]</sup>



RADIAL CONDUCTIVITY



AXIAL CONDUCTIVITY



# MODELLING WATER FLOW AT THE ORGAN SCALE

## - MECHA - <https://github.com/water-fluxes/day-2-organ-MECHA>

water-fluxes / day-2-organ-MECHA Public

<> Code Issues Pull requests Actions Projects Security Insights

main 1 branch 0 tags Go to file Code

HeymansAdrien update Ntot 4 hours ago 16 commits

GRANAR added granar files 27 days ago

MECHA Update MECHAv4\_light.py 5 hours ago

\_pycache\_ added mecha files 27 days ago

.DS\_Store added granar files 27 days ago

.Rhistory updated readme 27 days ago

LICENSE added mecha files 27 days ago

README.md updated readme 27 days ago

Run\_MECHA.ipynb update Ntot 4 hours ago

environment.yml added mecha files 27 days ago

install.R added R binder files 27 days ago

mecha.py added mecha files 27 days ago

mecha\_function.py update Ntot 4 hours ago

runtime.txt added R binder files 27 days ago

About Day 2 ~ MECHA

Readme GPL-3.0 license 0 stars 1 watching 0 forks

Contributors 3

guillaumelobet Guillaume Lobet

ValentinCouverreur

HeymansAdrien

Languages

Python 86.5% R 11.8% Jupyter Notebook 1.7%

README.md

Material for the day 2 of the summer school - Organ scale water flow in roots - MECHA

In this repository you will ressources to run MECHA

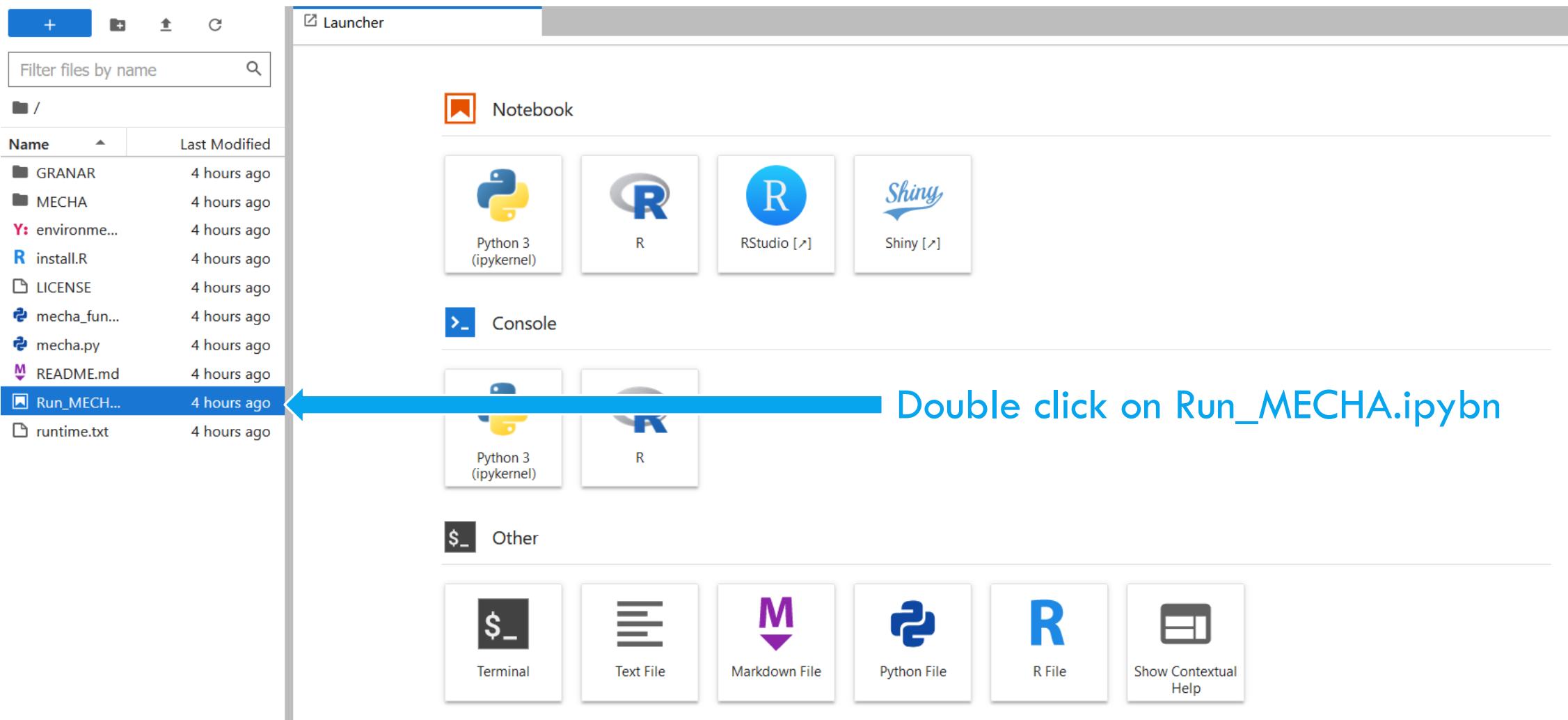
You can launch the notebook here : [Launch Binder](#)

Run MECHA via Binder

# MODELLING WATER FLOW AT THE ORGAN SCALE

## - MECHA -

Once on Binder... let's open the Jupyter Notebook!



# MODELLING WATER FLOW AT THE ORGAN SCALE

## - MECHA -

Once on Binder/Jupyter Notebook... let's run MECHA!

The screenshot shows a Jupyter Notebook interface with a sidebar containing file management tools and a list of XML files. The main area displays a code cell with Python code for running the MECHA model. A blue arrow points to the play button in the toolbar above the cell, with the text "2. Click on play". Another blue arrow points to the first line of code in the cell, with the text "1. Click on a cell". Two more blue arrows point to specific lines of output text, with the text "3.  $k_r$  for root with Casp" and "4.  $k_r$  for suberised root" respectively.

File Edit View Run Kernel Tabs Settings Help

+ Filter files by name

/ MECHA / cellsetdata /

Name	Last Modified
current_root.xml	a day ago
current_root_tap.xml	a day ago

Launcher Run\_MECHA.ipynb +

MECHA: Upon this generated cross-section and the cell hydraulic properties defined in Hydraulic.xml MECHA estimates the radial hydraulic conductivities (for three scenarios: 1 = an endodermal caspary strip, 2 = a fully suberized endodermis, 3 = fully suberized endodermis and a

2. Click on play

Change kernel to Python to launch the following script. Once the kernel is changed, all variables stored in R are gone.

```
[2]: from mecha_function import *
mecha()

Importing geometrical data
Import Geometrical data
Creating network nodes
Creating network connections
Importing hydraulic data
Maturity #0 with apoplastic barrier type #1
Radial conductivity: 0.00016366878594094897 cm/hPa/d
Maturity #1 with apoplastic barrier type #4
Radial conductivity: 4.794135423239936e-05 cm/hPa/d
End of mecha
```

1. Click on a cell

3.  $k_r$  for root with Casp

4.  $k_r$  for suberised root

# MODELLING WATER FLOW AT THE ORGAN SCALE

## - MECHA -

Let us check the root anatomies available...

The screenshot shows a software interface with a file explorer on the left and a code editor on the right.

**File Explorer:**

- File menu: File, Edit, View, Run, Kernel, Tabs, Settings, Help.
- Toolbar: +, Filter files by name, Up, Down, Refresh.
- Filter files by name: current\_root.xml, current\_root\_tap.xml.
- Folder: / MECHA / cellsetdata /
- Table: Name (current\_root.xml, current\_root\_tap.xml), Last Modified (a day ago).

**Code Editor:**

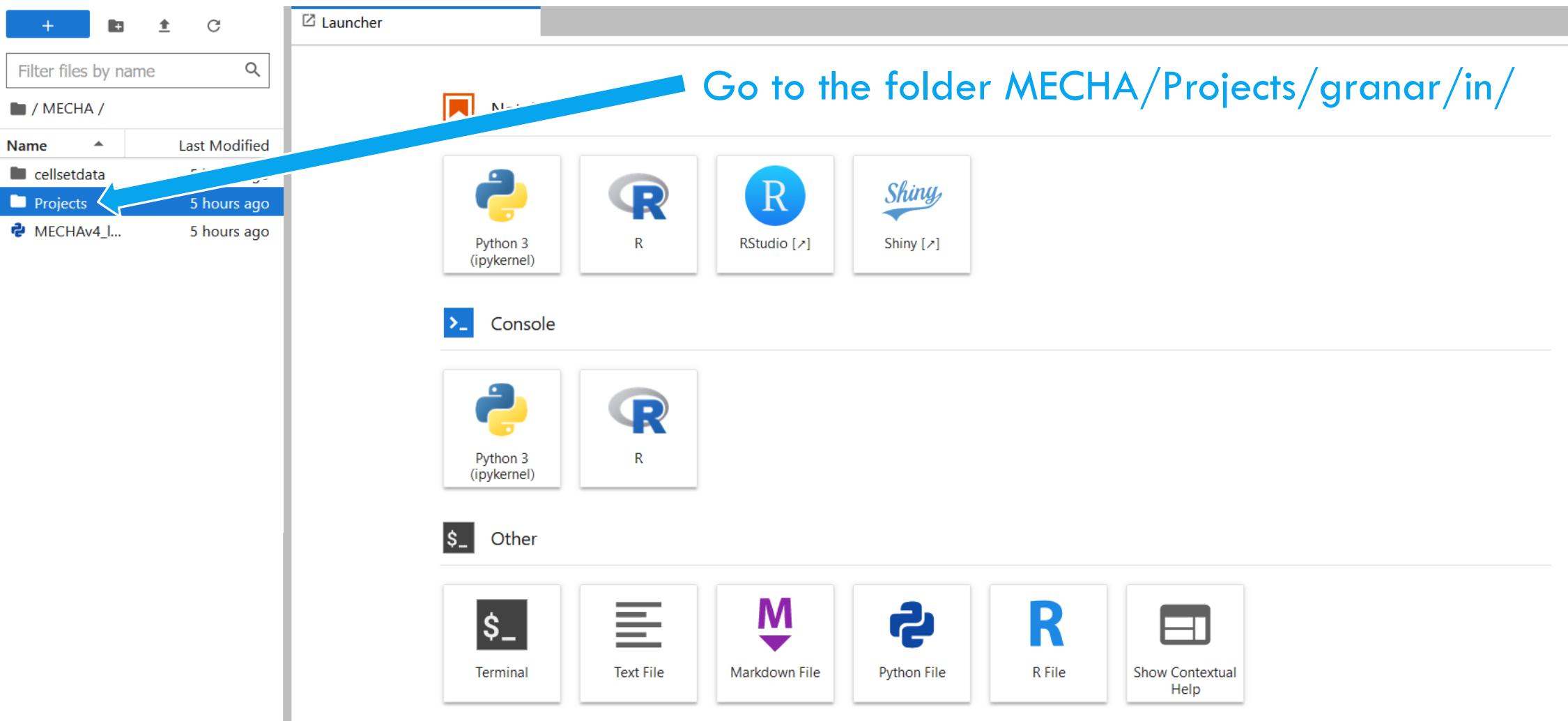
- Launcher tab: Run\_MECHA.ipynb, Maize\_Geometry\_aer.xml, current\_root.xml, current\_root\_tap.xml.
- Code (XML snippet):

```
60 <parameters>
61   <parameter io="output" name="stellar" type="layer_area" value="0.358809969692149"/>
62   <parameter io="output" name="cortex_alive_to_epidermis" type="layer_area" value="1.58328877011"/>
63   <parameter io="output" name="all" type="layer_area" value="1.94209873980215"/>
64 </parameters>
65 </metadata>
66 <cells count="853">
67   <cell id="0" group="5" truncated="false" >
68     <walls>
69       <wall id="0"/>
70       <wall id="1"/>
71       <wall id="2"/>
72       <wall id="3"/>
73       <wall id="4"/>
74     </walls>
75   </cell>
76   <cell id="1" group="5" truncated="false" >
77     <walls>
78       <wall id="5"/>
79       <wall id="6"/>
80       <wall id="7"/>
81       <wall id="8"/>
82       <wall id="9"/>
83     </walls>
84   </cell>
85   <cell id="2" group="5" truncated="false" >
86     <walls>
87       <wall id="10"/>
88       <wall id="11"/>
89       <wall id="12"/>
90       <wall id="13"/>
91     </walls>
92   </cell>
```

# MODELLING WATER FLOW AT THE ORGAN SCALE

- MECHA -

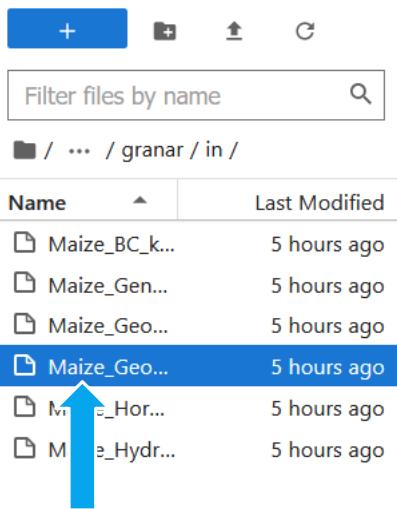
Once on Binder... let's update the root anatomy!



# MODELLING WATER FLOW AT THE ORGAN SCALE

## - MECHA -

Once on Binder... let's update the root anatomy!



1. Open the file  
'Maize\_geometry\_aer.xml'

```
<?xml version="1.0" encoding="utf-8"?>
<param>
    <!-- Plant type -->
    <Plant value='Root' /> <!-- Maize / Arabido / Millet / Barley /-->

    <!-- Image path and properties -->
    <path value='current_root.xml' />
    <im_scale value="1000" /> <!-- #image scale (micron per pixel) -->

    <!-- Maturity Level
    0: No apoplastic barriers
    1: Endodermal Casparyan strip (radial walls)
    2: Endodermal suberization except at passage cells
    3: Endodermis full suberization
    4: Endodermis full suberization and exodermal Casparyan strip (radial walls) -->
    <Maturityrange> <!-- All the listed barrier types will be simulated and reported in separate files "***b1",
    "***b2", "***b3", ... -->
        <Maturity Barrier="1" height="200" Nlayers="1"/>
        <Maturity Barrier="4" height="200" Nlayers="1"/>
    </Maturityrange>
    <Printrange>
        <Print_layer value="0"/>
    </Printrange>
    <Xwalls value="1" /> <!-- 0: No transverse walls in the 2D simulations; 1: Transverse walls included in 2D
    simulations -->
    <PileUp value="0" /> <!-- 0: Simulating different levels of maturity separately (2D); 1: Simulating all levels
    of maturity interconnected (3D) -->

    <!-- Topological info (passage cells and intercellular spaces) -->
    <passage_cell_range>
        <passage_cell id="-1" /> <!-- ID number of passage cells in the endodermis, ideally in front of early
        metaxylem vessels -->
    </passage_cell_range>
    <kaerenchyma_range>
```

3. Update the name of folder in which the new outputs will be stored
2. Update the name of the dragged GRANAR output, so it corresponds to your new root anatomy file name (e.g. 'current\_root\_tap.xml')

4. In Run\_MECHA.ipynb, run the cell « from mecha\_function ... » and check new kr values

# MODELLING WATER FLOW AT THE ORGAN SCALE

- MECHA -

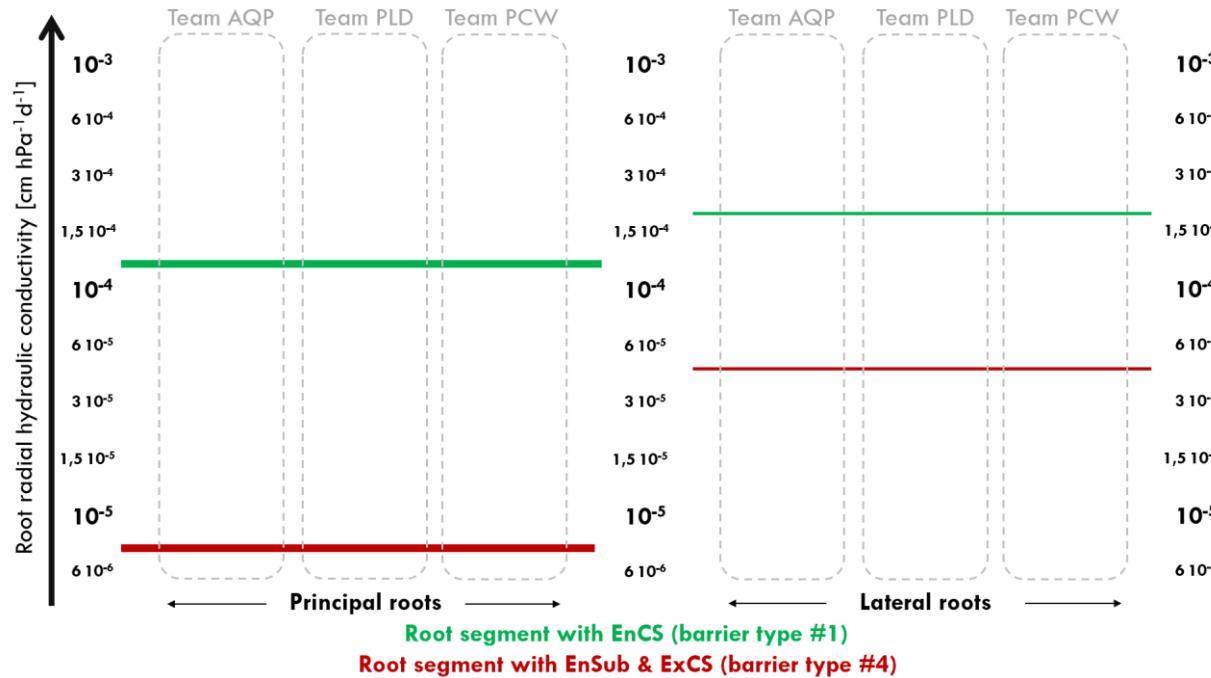
Once on Binder... let's update the cell hydraulic properties!

The screenshot shows a Jupyter Notebook interface with three tabs: 'Launcher', 'Run\_MECHA.ipynb', and 'Maize\_Hydraulics.xml'. The 'Maize\_Hydraulics.xml' tab displays an XML configuration file. The file browser on the left lists several XML files related to maize hydraulic scenarios. The 'Maize\_Hydraulics.xml' file contains code for setting hydraulic paths and parameters. A blue arrow points from the text '1. Open the file 'Maize\_hydraulics.xml'' to the file browser. Another blue arrow points from the text '2. Update the hydraulic conductivity of cell walls (kw) or membranes aquaporins (kAQP), or plasmodesmata (Kpl)' to the XML code. A third blue arrow points from the text '3. Update the name of the scenario' to the XML code.

```
<?xml version="1.0" encoding="UTF-8"?>
<!-- Hydraulic options -->
<param>
    <!-- Path to the folders of different hydraulic scenarios -->
    <path_hydraulics>
        <!-- By order of selected properties -->
        <Output path="baseline/" />
        <!--Output path='2.4E-04_4.3E-4/' />
        <Output path='1.2E-05_4.3E-4/' />
        <Output path='6.0E-06_6.8E-5/' />
        <Output path='1.2E-05_6.8E-5/' />
        <Output path='6.0E-06_6.8E-5/' /-->
    </path_hydraulics>
    <!-- Cell wall hydraulic conductivity
        Review in Transport in plants II: Part B Tissues and Organs, A. Lauchli: 1. Apoplastic transport in
        tissues
        Units: cm^2/hPa/d
        6.6E-03: Soybean hypocotyl Steudle and Boyer (1985)
        2.4E-04: Zhu and Steudle (1991)
        1.2E-05: Nitella cell Tyree (1968)
        6.0E-06: Nitella cell walls Zimmermann and Steudle (1975)
        1.3E-07: Cellulose wall Briggs (1967) for thickness of 1.5 micron
        1.8E-09: Maize root cell wall Tyree (1973) for thickness of 1.5 micron -->
    <kwrange>
        <kw value="0.000024"/>
```

4. In Run\_MECHA.ipynb, run the cell « from mecha\_function ... » and check new kr values

# Add updates radial conductivities in your team's column !



1

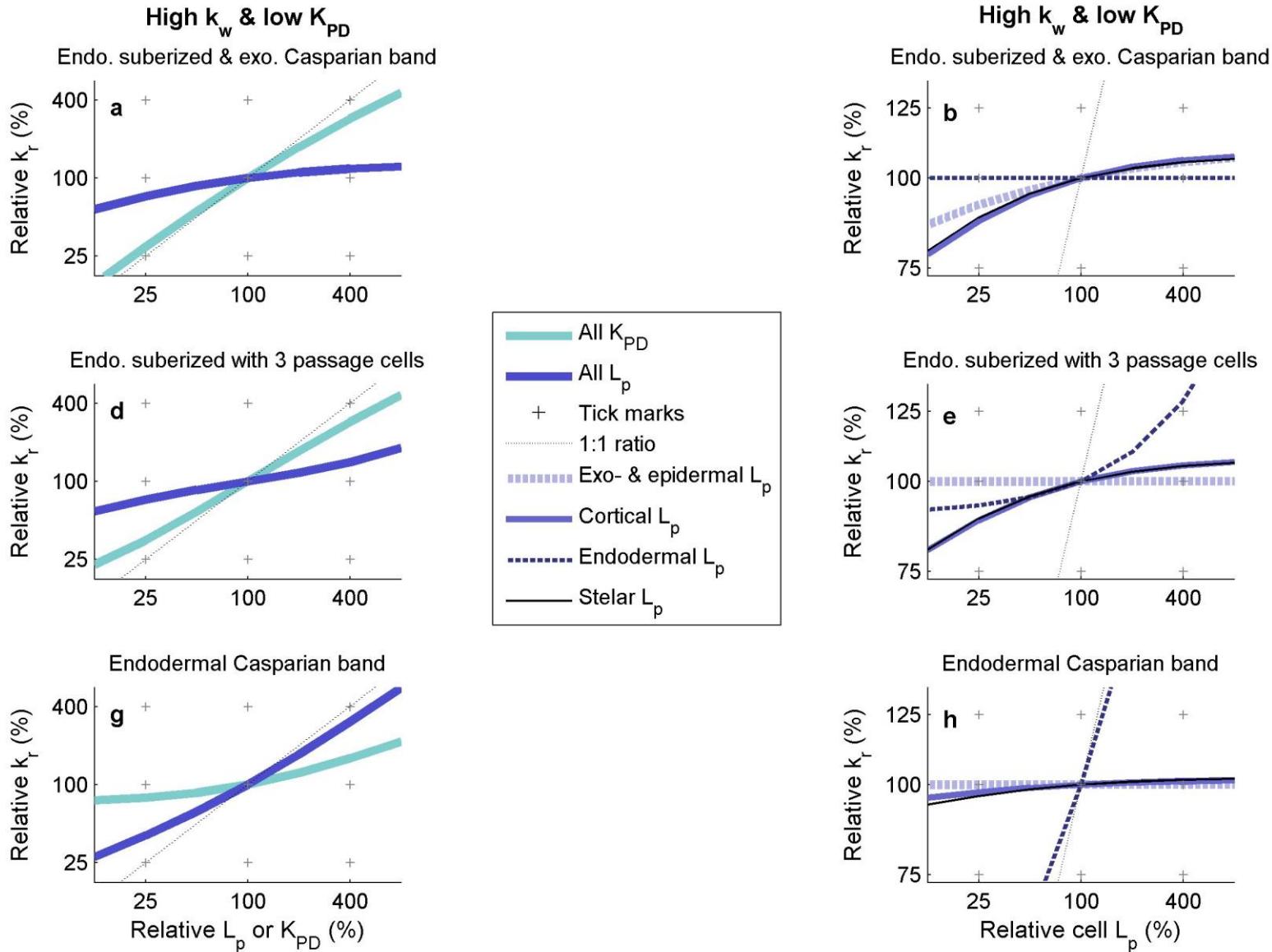
Allez sur [wooclap.com](https://wooclap.com)

2

Entrez le code d'événement dans le bandeau supérieur

Code d'événement  
**MECHA2219**

# SENSITIVITY ANALYSIS



# MODELLING WATER FLOW AT THE ORGAN SCALE

- MECHA -

<https://plantmodelling.shinyapps.io/mecha/>

Valentin Couvreur, Marc Faget, Guillaume Lobet, Mathieu Javaux, François Chaumont and Xavier Draye

Université catholique de Louvain, Forschungszentrum Juelich GmbH

Choose plant Change parameters About

Choose a simulation to visualize

1. Select a plant type

Arabidopsis1

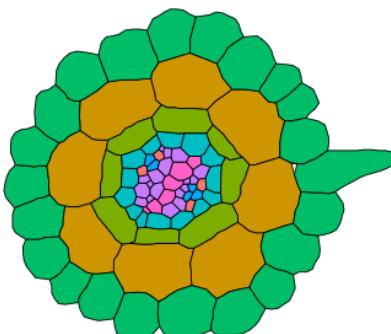
MECHA was run for different cross section geometries and plant type. The results were pre-processed to be easily visualised here.

**UCL**  
Université  
catholique  
de Louvain

**JÜLICH**  
FORSCHUNGSZENTRUM

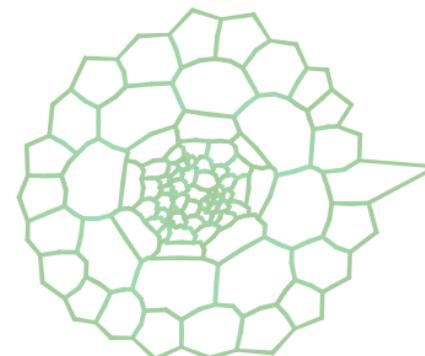
## Tissue layers

Visualisation of the different cell layers used in the simulation



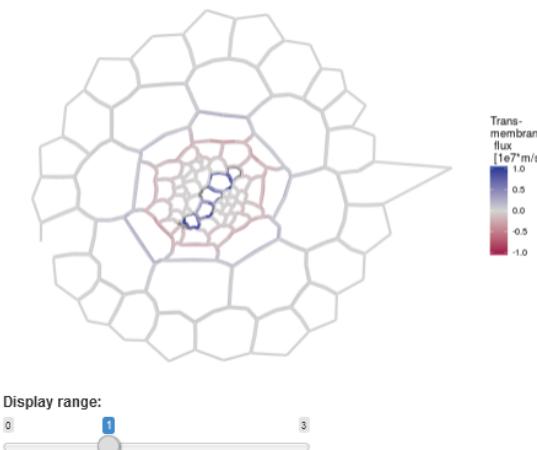
## Cell walls fluxes

Flows with the cell walls of the cross section.



## Transmembrane fluxes

Flows with the cell membranes of the cross section. Blue color indicates when the water is entering the cell. Red color indicates when the water is leaving the cell.



Select the information to visualize

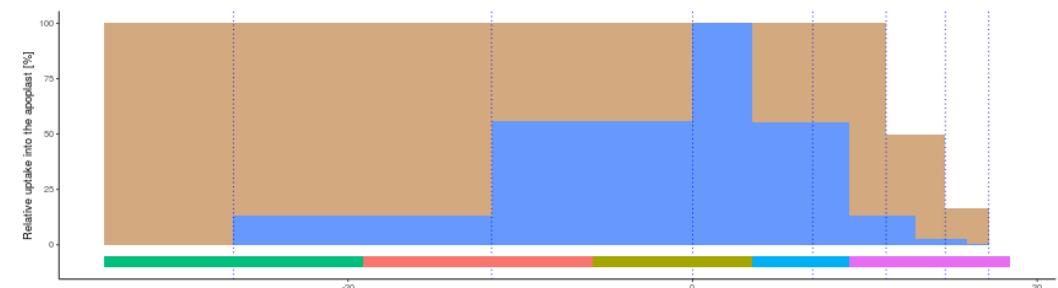
fluxes

Synthetic information about the simulation

param	value	unit
Cross-section height	0.01	cm
Cross-section perimeter	0.0304	cm
Cross-section radial conductivity	2.47e-04	cm/hPa/d
Xylem pressure potential	1100	hPa
Soil pressure potential	-100	hPa
Xylem osmotic potential	-1500	hPa
Soil osmotic potential	-200	to
Soil contact	0e+00	microns
Wall conductivity	0.0066	cm^2/hPa/d
Plasmodesmata conductivity	3.1e-11	cm^3/hPa/d
Aquaporin conductivity	4.3e-04	cm/hPa/d

## Relative contribution of water pathways

Visualisation of the relative contribution of the apoplastic and symplastic pathways to the global water flow across the root cross-section



- Modelling Root Radial Hydraulics -

**UCLouvain**