



THE 1ST INTERNATIONAL SUMMER SCHOOL ON ADVANCED SOIL PHYSICS

MODELING WATER FLUXES IN THE SOIL-PLANT SYSTEM

MODELLING ROOT μ HYDRAULICS - MECHA

VALENTIN COUVREUR

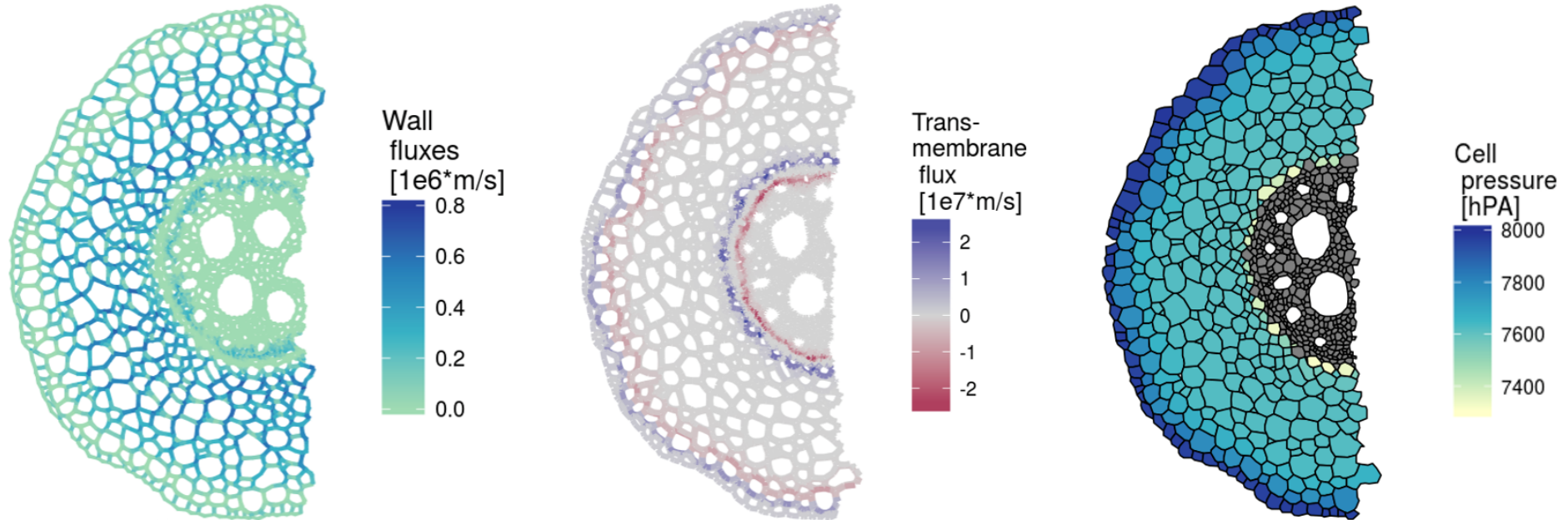
 **UCLouvain**



ENVITAM

MODELLING WATER FLOW AT THE ORGAN SCALE

- MECHA -



 Open Source

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



RADIAL CONDUCTIVITY



AXIAL CONDUCTIVITY

Couvreur V, Faget M, Lobet G, Javaux M, Chaumont F, Draye X, Going with the Flow: Multiscale Insights into the Composite Nature of Water Transport in Roots, *Plant Physiology*, Volume 178, Issue 4, December 2018, Pages 1689–1703, <https://doi.org/10.1104/pp.18.01006>

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

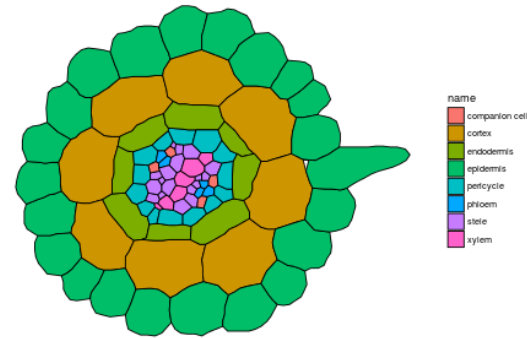
MECHA was run for different cross section geometries and plant type. Te results were pre-processed to be easily visualised here.

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de Louvain

JÜLICH
FORSCHUNGSZENTRUM

Tissue layers

Visualisation of the different cell layers used in the simulation



Select the information to visualize

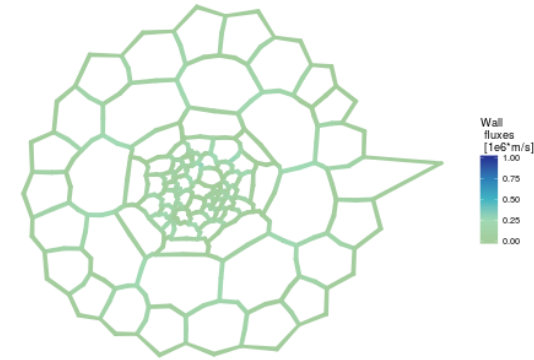
fluxes

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

Cell walls fluxes

Flows with the cell walls of the cross section.

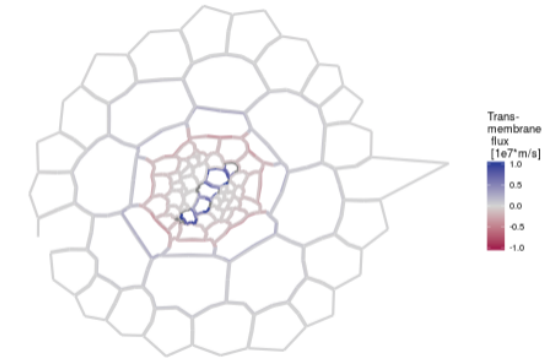


Display range:



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.

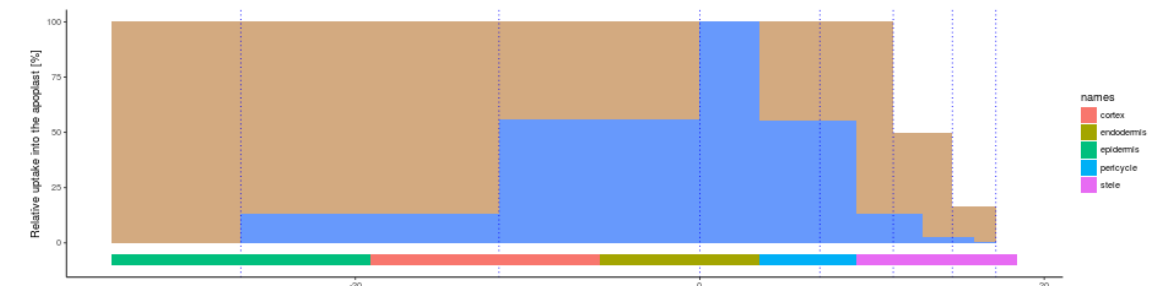


Display range:



Relative contribution of water pathways

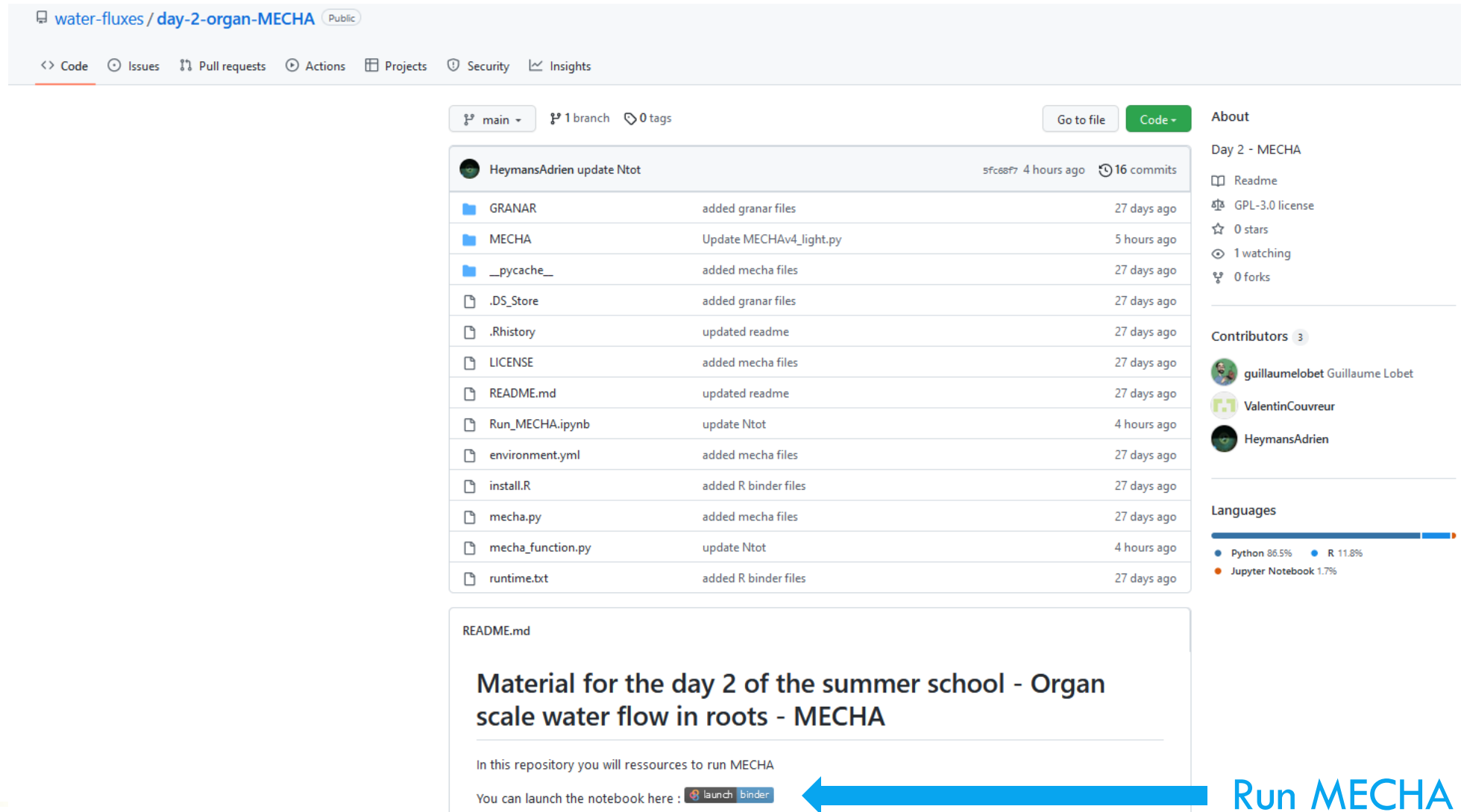
Visualisation of the relative contribution of the apolastic and symplastic pathways to the global water flow across the root cross-section



MODELLING WATER FLOW AT THE ORGAN SCALE

- MECHA -

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



The screenshot shows the GitHub repository page for 'water-fluxes/day-2-organ-MECHA'. The repository is public and has 16 commits. The commit history table lists the following files and their update times:

File	Commit Message	Time Ago
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

The README.md file contains the following text:

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

In this repository you will find resources to run MECHA

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

The right sidebar shows the repository's metadata: 0 stars, 1 watching, 0 forks. The contributors list includes guillaumelobet, ValentinCouvreur, and HeymansAdrien. The languages section shows Python (86.5%), R (11.8%), and Jupyter Notebook (1.7%).

Run MECHA via Binder

MODELLING WATER FLOW AT THE ORGAN SCALE

- MECHA -

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

The screenshot shows the Binder Launcher interface. On the left is a file browser with a search bar and a list of files. The file 'Run_MECHA.ipynb' is highlighted with a blue arrow pointing to it from the right. The main area shows three sections: 'Notebook' with icons for Python 3 (ipykernel), R, RStudio, and Shiny; 'Console' with icons for Python 3 (ipykernel) and R; and 'Other' with icons for Terminal, Text File, Markdown File, Python File, R File, and Show Contextual Help.

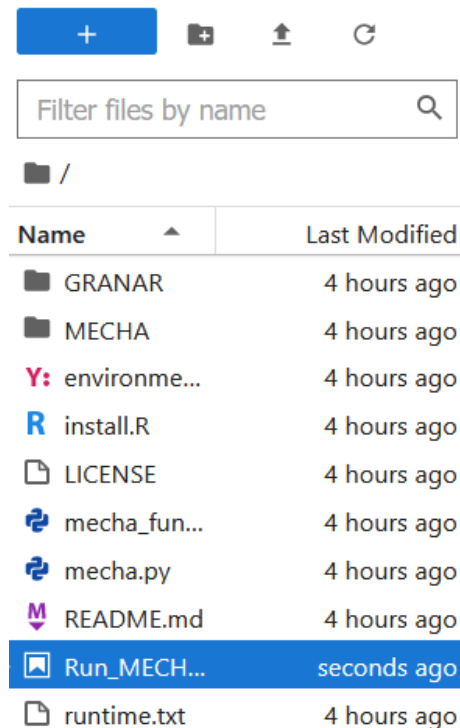
Name	Last Modified
GRANAR	4 hours ago
MECHA	4 hours ago
Y: environme...	4 hours ago
R install.R	4 hours ago
LICENSE	4 hours ago
mecha_fun...	4 hours ago
mecha.py	4 hours ago
README.md	4 hours ago
Run_MECHA...	4 hours ago
runtime.txt	4 hours ago

Double click on Run_MECHA.ipynb

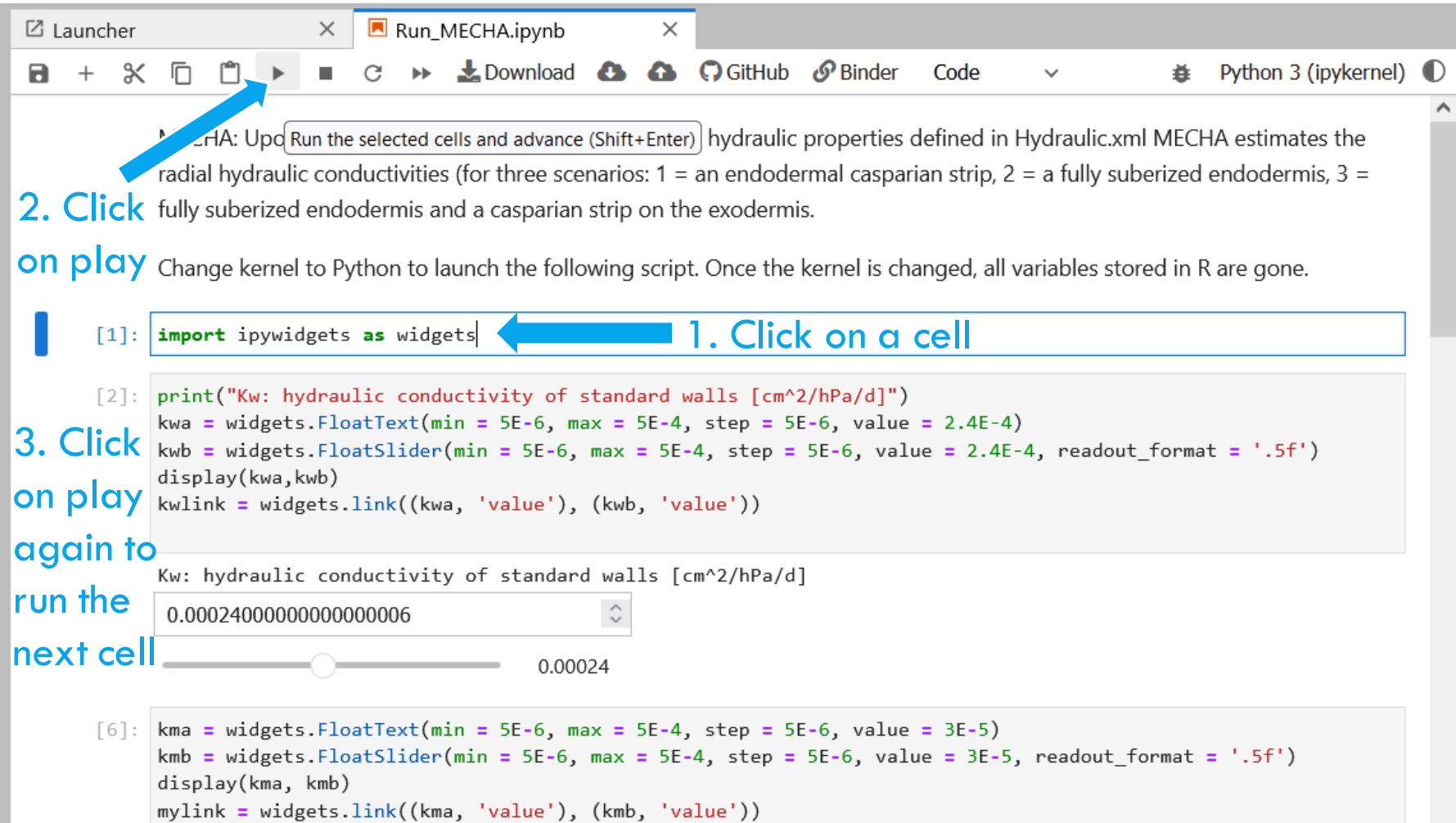
MODELLING WATER FLOW AT THE ORGAN SCALE

- MECHA -

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



Name	Last Modified
GRANAR	4 hours ago
MECHA	4 hours ago
Y: environme...	4 hours ago
R install.R	4 hours ago
LICENSE	4 hours ago
mecha_fun...	4 hours ago
mecha.py	4 hours ago
README.md	4 hours ago
Run_MECH...	seconds ago
runtime.txt	4 hours ago



1. Click on a cell

```
[1]: import ipywidgets as widgets
```

2. Click on play

```
[2]: print("Kw: hydraulic conductivity of standard walls [cm^2/hPa/d]")
kwa = widgets.FloatText(min = 5E-6, max = 5E-4, step = 5E-6, value = 2.4E-4)
kwb = widgets.FloatSlider(min = 5E-6, max = 5E-4, step = 5E-6, value = 2.4E-4, readout_format = '.5f')
display(kwa,kwb)
kwlink = widgets.link((kwa, 'value'), (kwb, 'value'))
```

3. Click on play again to run the next cell

```
[6]: kma = widgets.FloatText(min = 5E-6, max = 5E-4, step = 5E-6, value = 3E-5)
kmb = widgets.FloatSlider(min = 5E-6, max = 5E-4, step = 5E-6, value = 3E-5, readout_format = '.5f')
display(kma, kmb)
mylink = widgets.link((kma, 'value'), (kmb, 'value'))
```

4. As a starter, run the script with default kwa and kma values. It'll take a few min.

MODELLING WATER FLOW AT THE ORGAN SCALE

- MECHA -

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

File Edit View Run Kernel Tabs Settings Help

Filter files by name

/

Name	Last Modified
GRANAR	6 hours ago
MECHA	6 hours ago
environment.yml	6 hours ago
install.R	6 hours ago
LICENSE	6 hours ago
mecha_function.py	6 hours ago
mecha.py	6 hours ago
README.md	6 hours ago
Run_MECHA.ipynb	3 minutes ago
runtime.txt	6 hours ago

Launcher Run_MECHA.ipynb Maize_Geometry.xml

Download GitHub Binder Code

```
kmb = widgets.FloatSlider(min = 5E-6, max = 5E-4, step = 5E-6, value = 3E-5, readout_format = '.5f')
display(kmb)
mylink = widgets.link((kmb, 'value'), (kmb, 'value'))
```

0,00003

0.00003

```
[4]: kw = kwa.value
      km = kma.value
```

```
[5]: 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: 0.00016366878594094685 cm/hPa/d
Maturity #1 with apoplastic barrier type #4
Radial conductivity: 4.794135423239589e-05 cm/hPa/d
End of mecha

1. k_r for root with Casp

2. k_r for suberised root

MODELLING WATER FLOW AT THE ORGAN SCALE

- MECHA -

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

The screenshot shows the Binder interface. On the left is a file explorer with a search bar and a list of files and folders. The 'MECHA' folder is highlighted with a blue arrow. On the right is the 'Launcher' section with three tabs: 'Notebook', 'Console', and 'Other'. The 'Notebook' tab is active and shows four options: Python 3 (ipykernel), R, RStudio [↗], and Shiny [↗]. The 'Console' tab shows two options: Python 3 (ipykernel) and R. The 'Other' tab shows six options: Terminal, Text File, Markdown File, Python File, R File, and Show Contextual Help.

Filter files by name

Name Last Modified

GRANAR

MECHA 5 hours ago

environment.yml 5 hours ago

install.R 5 hours ago

LICENSE 5 hours ago

mecha_function.py 5 hours ago

mecha.py 5 hours ago

README.md 5 hours ago

Run_MECHA.ipynb 3 minutes ago

runtime.txt 5 hours ago

Launcher

Notebook

Python 3 (ipykernel)

R

RStudio [↗]

Shiny [↗]

Console

Python 3 (ipykernel)

R

Other

Terminal

Text File

Markdown File

Python File

R File

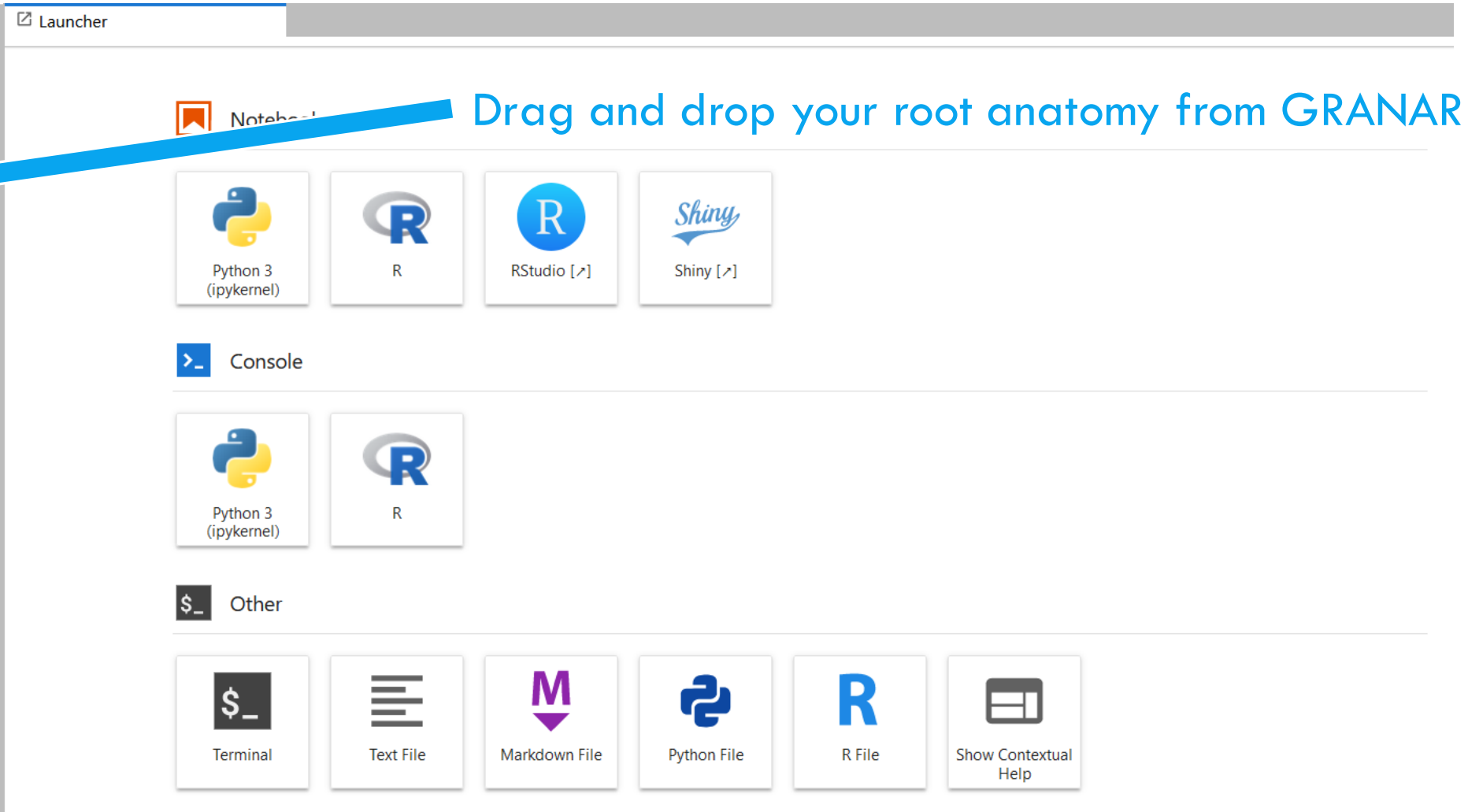
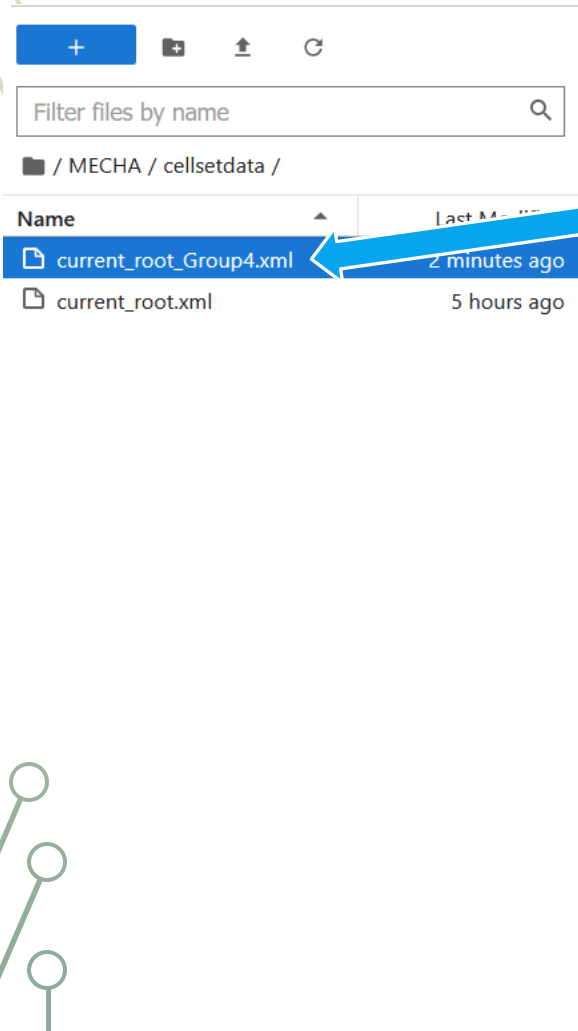
Show Contextual Help

Double click on folders MECHA/ then cellsetdata/

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!

Filter files by name

/ MECHA /

Name	Last Modified
cellsetdata	5 hours ago
Projects	5 hours ago
MECHAv4_l...	5 hours ago

Go to the folder `MECHA/Projects/granar/in/`

Launcher

Python 3 (ipykernel)

R

RStudio [↗]

Shiny [↗]

Console

Python 3 (ipykernel)

R

Other

Terminal

Text File

Markdown File

Python File

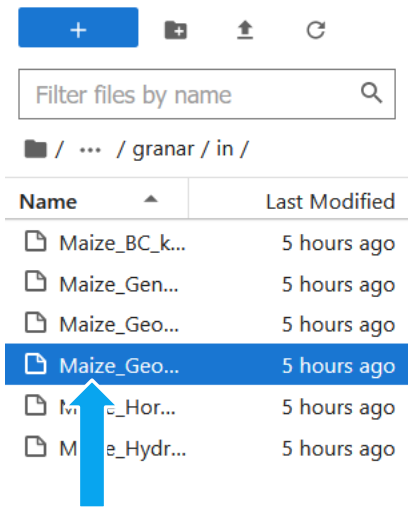
R File

Show Contextual Help

MODELLING WATER FLOW AT THE ORGAN SCALE

- MECHA -

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



1. Open the file
'Maize_geometry.xml'

```
Launcher Run_MECHA.ipynb Maize_Geometry.xml
1 <?xml version="1.0" encoding="utf-8"?>
2
3 <param>
4   <!-- Plant type -->
5   <Plant value='Root' ...--#Maize / Arabido / Millet / Barley /-->
6
7   <!-- Image path and properties -->
8   <path value='current_root.xml' />
9   <im_scale value="1000" /> <!-- #image scale (micron per pixel) -->
10
11   <!-- Maturity Level
12   0: No apoplastic barriers
13   1: Endodermal Casparian strip (radial walls)
14   2: Endodermal suberization except at passage cells
15   3: Endodermis full suberization
16   4: Endodermis full suberization and exodermal Casparian strip (radial walls) -->
17   <Maturityrange> <!-- All the listed barrier types will be simulated and reported in separate files "b1",
18   "b2", "b3",... -->
19   <Maturity Barrier="1" height="200" Nlayers="1"/>
20   <Maturity Barrier="4" height="200" Nlayers="1"/>
21   </Maturityrange>
22   <Printrange>
23   <Print_layer value="0"/>
24   </Printrange>
25   <Xwalls value="1" /> <!-- 0: No transverse walls in the 2D simulations; 1: Transverse walls included in 2D
26   simulations -->
27   <PileUp value="0" /> <!-- 0: Simulating different levels of maturity separately (2D); 1: Simulating all levels
28   of maturity interconnected (3D) -->
29
30   <!-- Topological info (passage cells and intercellular spaces) -->
31   <passage_cell_range>
32     <passage_cell id="-1" /> <!-- ID number of passage cells in the endodermis, ideally in front of early
33     metaxylem vessels -->
34   </passage_cell_range>
35   <aerenchyma_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_Group4.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!

Filter files by name

/ ... / granar / in /

Name	Last Modified
Maize_BC_k...	6 hours ago
Maize_Gen...	6 hours ago
Maize_Geo...	6 hours ago
Maize_Geo...	6 hours ago
Maize_Hor...	6 hours ago
Maize_Hydr...	minutes ago

```
<?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: ... / kw / Kpd / kAQP -->
    <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-7: Cellulose wall Briggs (1967) for thickness of 1.5 micron
  1.8E-9: Maize root cell wall Tyree (1973) for thickness of 1.5 micron -->
  <kwrange>
    <kw value="0.000024"/>
```

3. Update the name of the scenario

1. Open the file 'Maize_hydraulics.xml'

2. Update the hydraulic conductivity of cell walls (kw) or membranes aquaporins (kAQP), lower in the file

4. In Run_MECHA.ipynb, run the cell « from mecha_function ... » and check new kr values

EXERCISE

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

- Please send your GRANAR inputs / outputs and MECHA kr values for default cell hydraulic properties to guillaume.lobet@uclouvain.be so we could discuss and compare anatomies and conductivities 😊