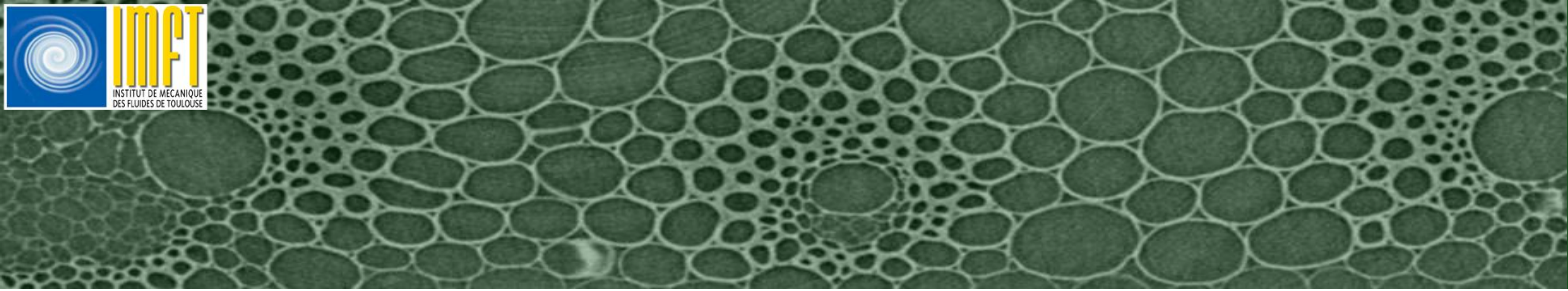


Multiscale modelling of enzymatic hydrolysis of biomass using numerical homogenisation

21 may 2026

Emma BERSON

Paul DURU, Pauline ASSEMAT

Porous and Biological Media group (Toulouse Fluid Mechanics Institute)

National project **Biomass, biotechnology and sustainable technologies for chemicals and fuels** (PEPR B-Best)

- Biomass = all organic matter that can be used as a source of energy

Sub-project **FillingGaps**: (9 partners from 6 institutions, 3.6M€ in funding over 2023-2027)

Objective: Develop multi-scale approaches to identify markers of biomass properties and reactivity to **enzymatic hydrolysis**

- Development of characterization tools at complementary scales. Integration of information, proposal of virtual models
- Improvement in process efficiency

Biomass of interest: unused agricultural residues (lignocellulosic biomass)

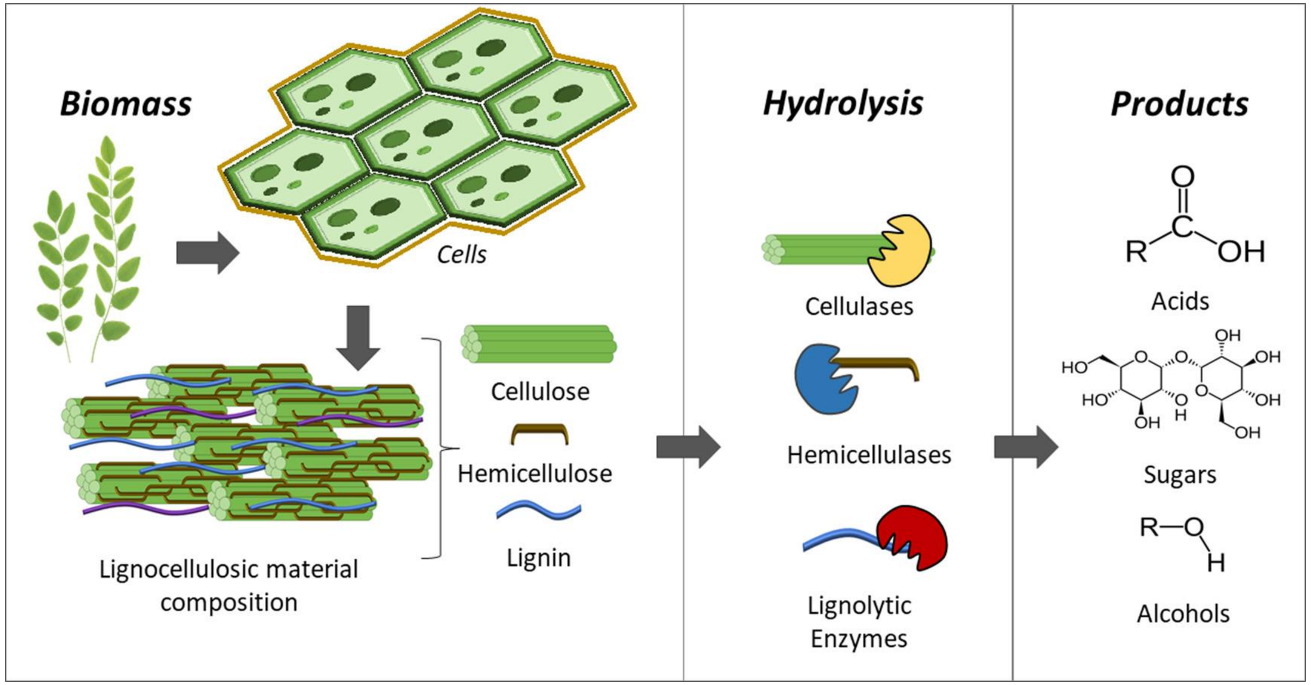
Some key figures:

- Lignocellulosic biomass accounts 50% in yearly worldwide biomass production
- Lignocellulosic biomass, an abundant resource: global production of 181 billion tons of waste per year[1]
- However, total global biomass remains underexploited (10%) for biofuel production

[1] M.K. Awasthi et al, Fuel, 2023

Enzymatic hydrolysis
degradation of biomass (usually crushed) by the action of enzymes in an aqueous medium

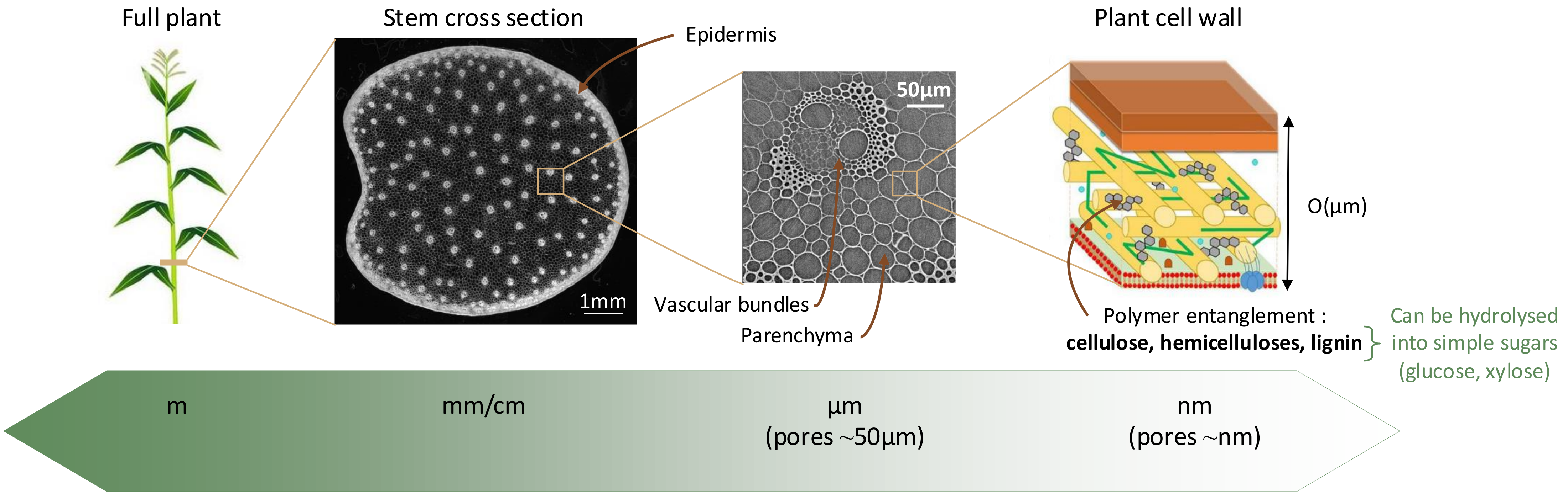
- Glucose and other products converted into energy (e.g. ethanol after fermentation), basic chemicals or bio-based materials
- Low-carbon energy source (low GHG emissions)



Saldarriaga-Hernandez et al., International Journal of Macromolecules, 2020

Maize, a complex porous medium

- Structural **heterogeneities** (parenchyma, bundles, epidermis) and chemical **heterogeneities** (cell wall composition)

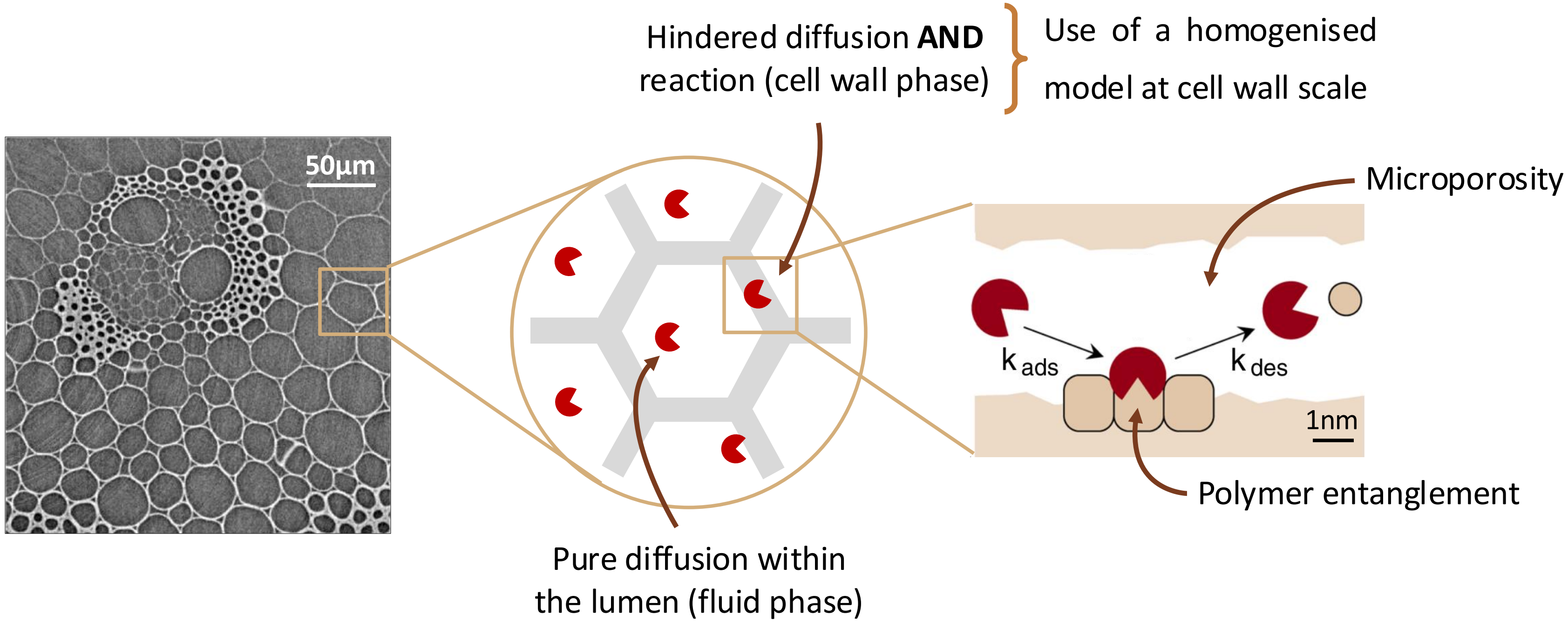


Adapted from Christophe Loix et al., Frontiers in Plant Science, 2018

- **Double porosity** medium

Objectives: Modelling enzymatic hydrolysis at the level of a maize fragment/section

- Diffusion/reaction problem in porous media



Methodology: Theoretical upscaling

Purely diffusive problem

Cell-scale L_1

diffusive flux → $\mathbf{J}$; diffusion tensor → $\mathbf{D}$; enzyme concentration → c

$$\begin{cases} \mathbf{J} = -\mathbf{D} \cdot \nabla c, \text{ on } \Omega \\ \nabla \cdot \mathbf{J} = 0, \text{ on } \Omega \\ \text{BCs on } \partial\Omega \end{cases}$$

$\mathbf{D}_0$: diffusion tensor of free enzymes in solution

$\mathbf{D}_P$: equivalent diffusion tensor in cell walls

Homogenisation by volume averaging[1]

Meso-scale L_2

For the new domain $\tilde{\Omega}$

diffusive flux at L_2-scale → $\tilde{\mathbf{J}}$; piecewise constant equivalent diffusion tensor → $\tilde{\mathbf{D}}(s)$; enzyme concentration at L_2-scale → $\tilde{c}$

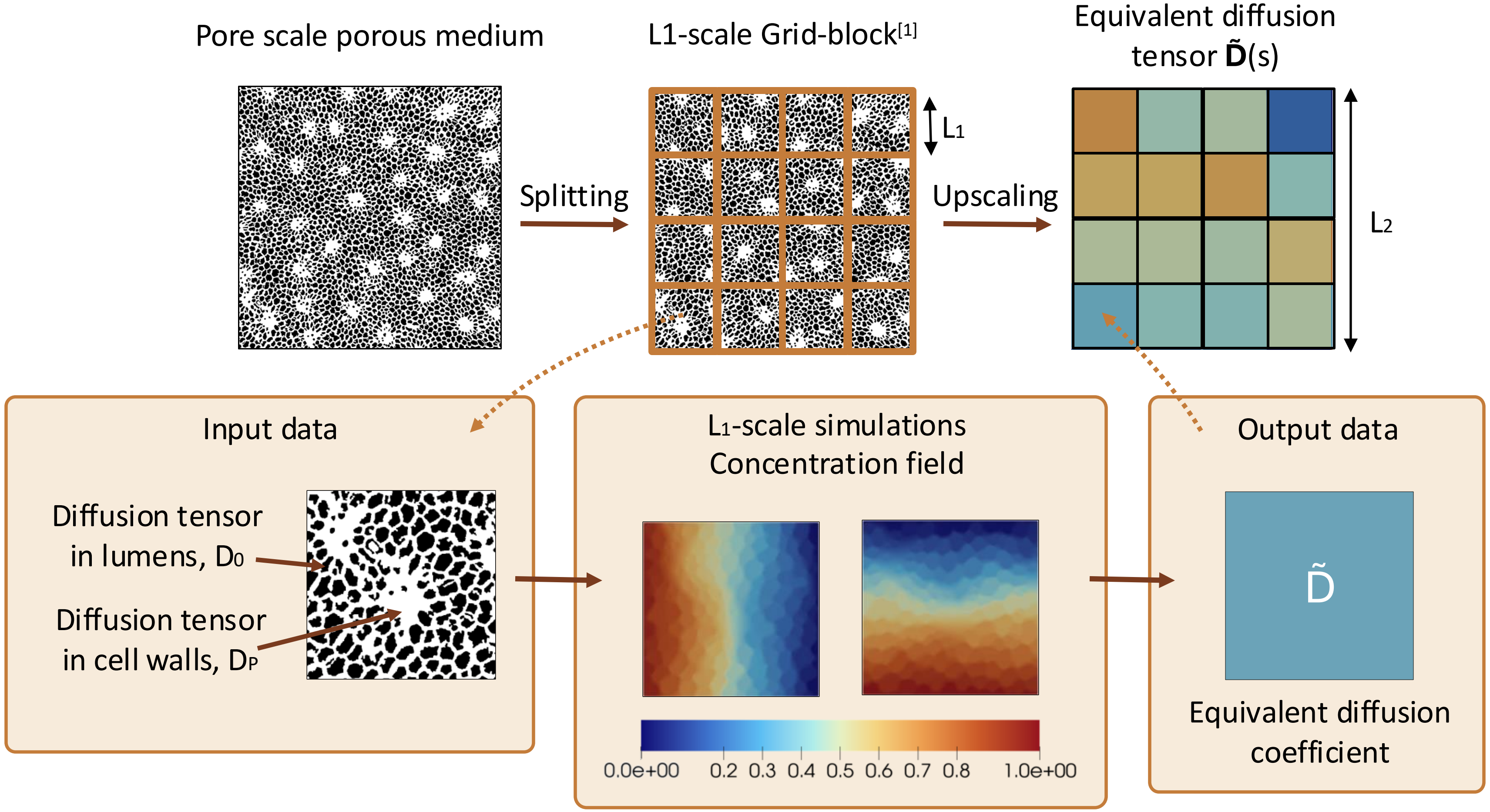
$$\begin{cases} \tilde{\mathbf{J}} = -\tilde{\mathbf{D}}(s) \cdot \nabla \tilde{c}, \text{ on } \tilde{\Omega} \\ \nabla \cdot \tilde{\mathbf{J}} = 0, \text{ on } \tilde{\Omega} \\ \text{BCs on } \partial\tilde{\Omega} \end{cases}$$

averaged flux from cell-scale simulation → $\langle \mathbf{J}_j \rangle^i$; characteristic length L_1 → L_1; imposed concentration gradient → $(\delta C)^i$

$$(\tilde{\mathbf{D}})_{ij} = \left(-\langle \mathbf{J}_j \rangle^i \frac{L_1}{(\delta C)^i} \right)_{1 \le i,j \le 2}$$

[1] S. Whitaker, transport In Porous Media, 1986

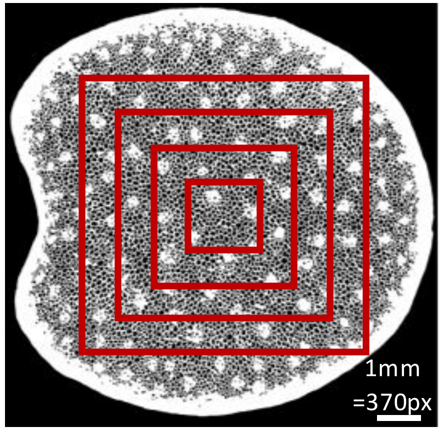
Methodology: Numerical homogenisation with Tumupscale code



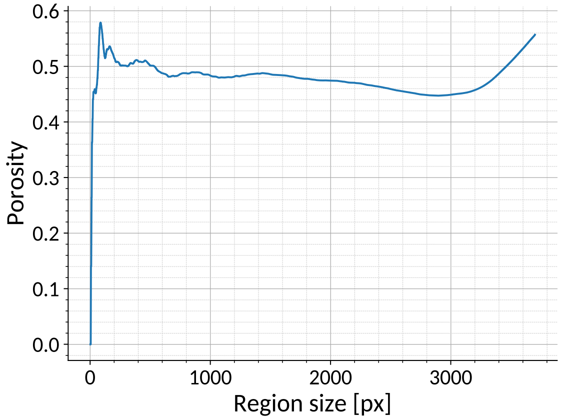
- Developed in Python, uses FeniCSx (finite element framework) and GMSH for the mesh
- Two validation codes: version in Julia (GridAp) and Comsol

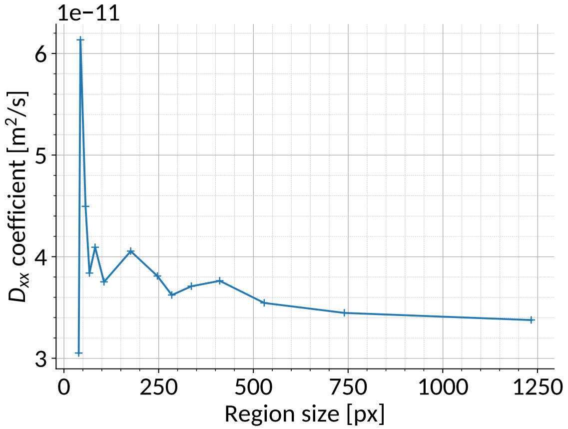
[1] L. Durlofsky, Water Rescources Research, 1991

- Methods applicable on porous media with no scale separation



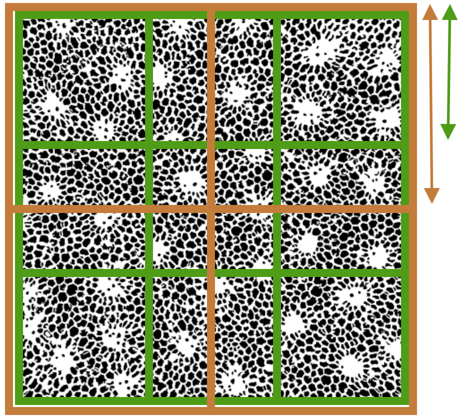
Binarised maize stem section





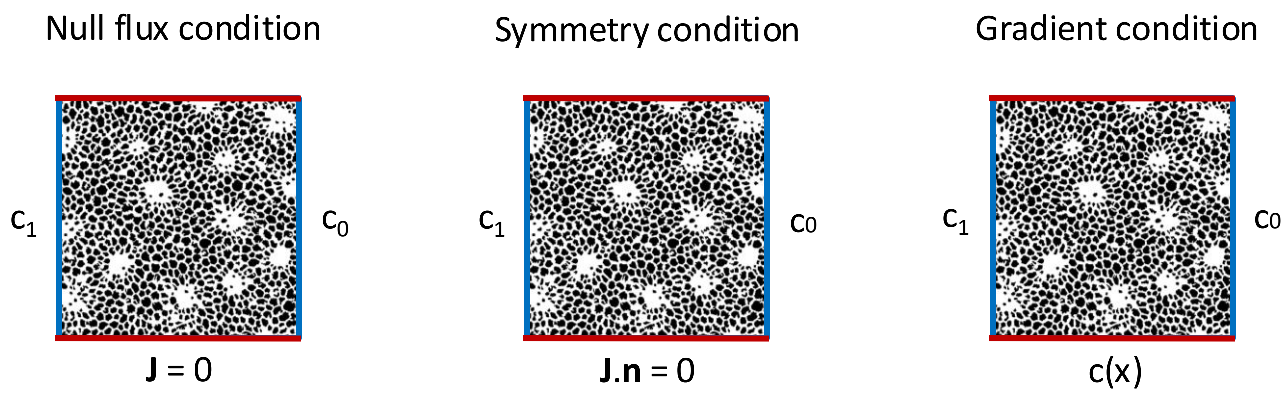
- In our case : pseudo plateaus ?

- Size L1 of the grid sub-domains
  - Arbitrary length, chosen to be equal to the size of the REV if there is a scale separation

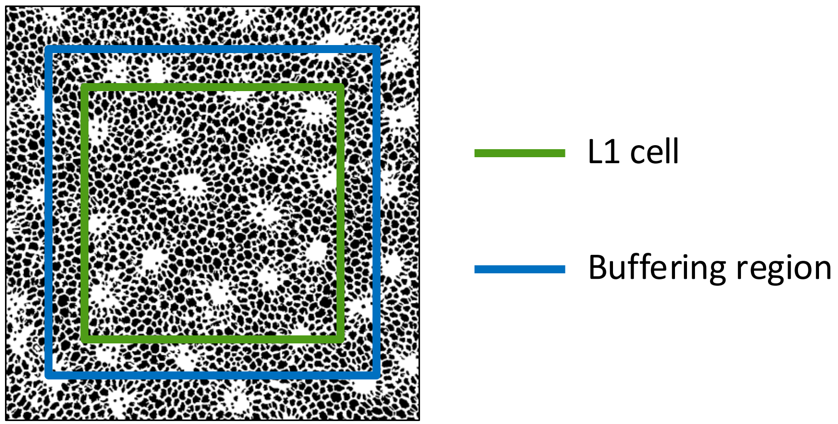


[1] L. Durlofsky, Water Rescources Research, 1991

- Tested boundary conditions:

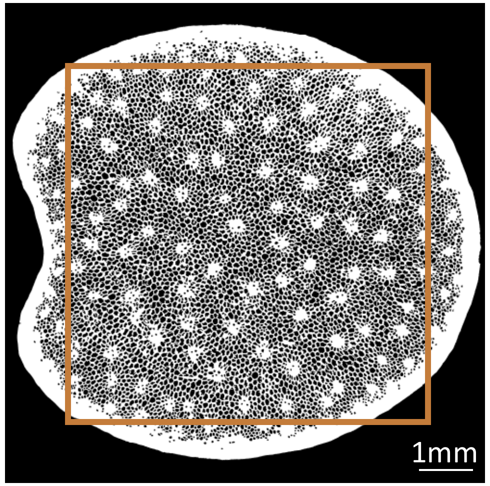


- Extend-local method
  - Push the boundary conditions further away (buffering region)



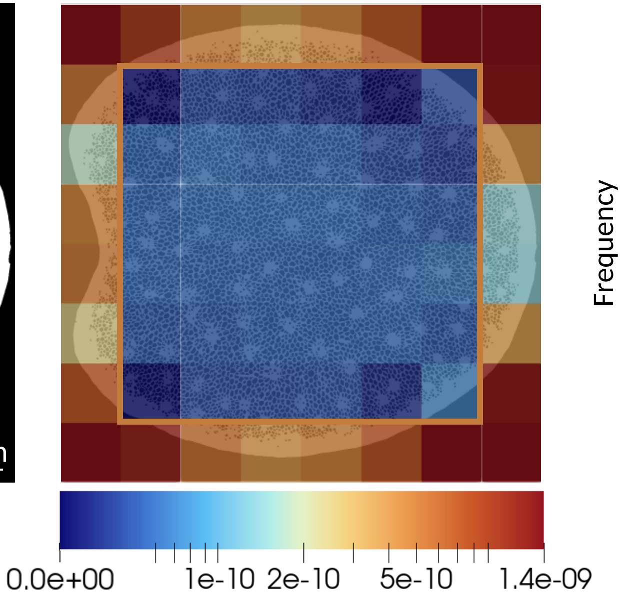
Equivalent coefficient maps

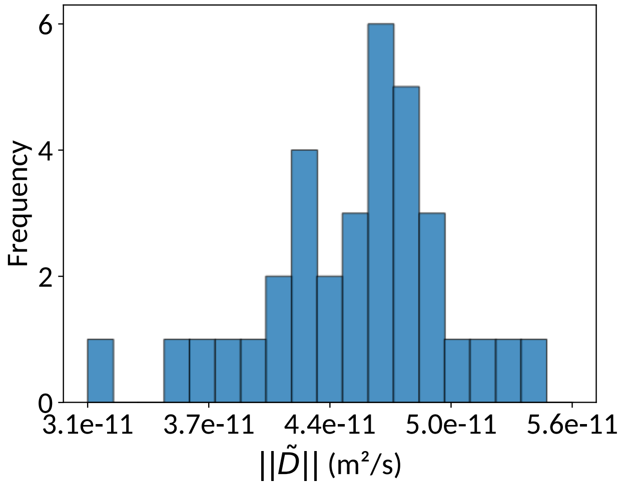
- Distribution of values on 2D images of biomass
    - cross-correlations: Deq values/location in biomass



Binarised maize stem section

Map of $||\tilde{D}||$ [m²/s]



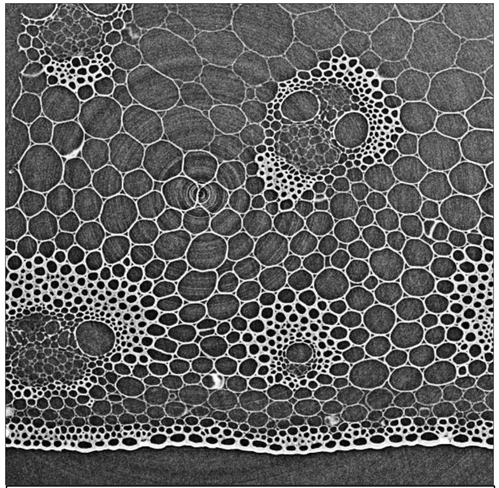


- $\tilde{D}$ value is controlled by the value set for D_P
- D_0= 10e-9 m^2/s
- D_P= 10e-11 m^2/s

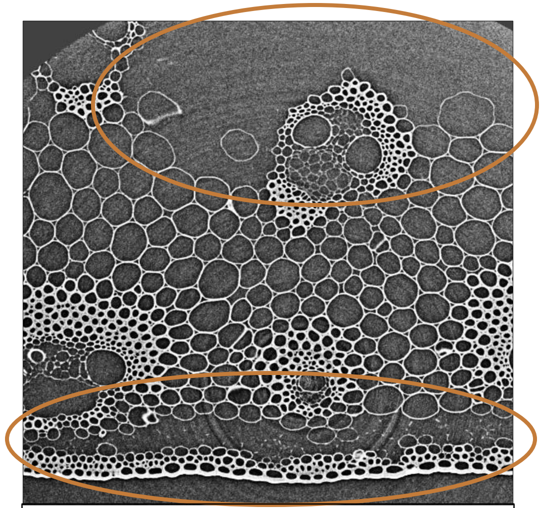
- Study of various samples with variable characteristics: different genotypes, structures, chemical composition and hydric conditions

Conclusion and perspectives

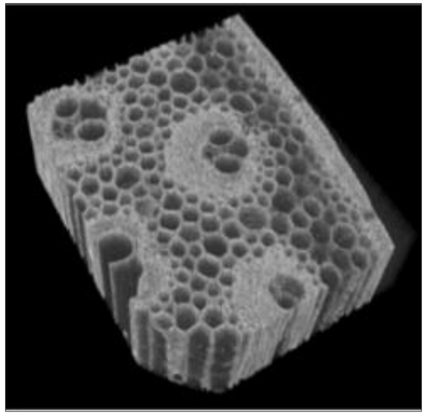
- Tools developed and operational for diffusion, currently implementing temporal and reactive aspects
- In terms of digital technology: 3D meshes, difficulties in capturing boundary conditions

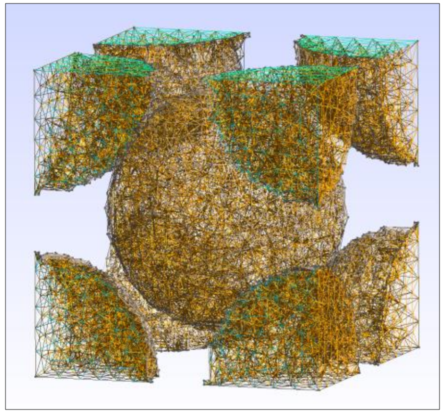


Native maize sample, T=0H
X-Ray tomography Soleil synchrotron



Enzymatic hydrolysis of the same sample, T=8H





Towards a 3D problem
(left) Soleil tomography
(right) 3D mesh generation test with GMSH on a stack of spheres