CIEM1110-1: Numerical modeling, lecture 1.1

Introduction to the unit

Frans van der Meer, Iuri Rocha

TU Delft

Welcome to module A: Measuring and modelling construction material behaviour

Two units:

- Numerical modeling of construction materials
- Experimental characterization of construction materials

Three assessments:

- Exam on *Numerical modeling*
- Exam on *Experimental characterization*
- Assignment portfolio covering both units

Three case studies (each with measuring and modeling):

- Concrete microstructure
- Viscoelasticity in bitumen
- Fracture of a mortar beam

Assignment portfolio

Three case studies, each involving measuring and modeling

- Work in groups of 3 and 2
  → join a group on brightspace under 'Collaboration'
- Follow the templates provided
  → they will be released one by one
- Intermediate deadlines weeks 4, 5 and 6
  → receive feedback on separate parts
- Final deadline Tuesday April 2 (week 8)
  → submit all reports on brightspace in a single pdf
- Presentations on Thursday April 4
  → every group presents about measuring and modeling for 1 of the 3 cases
  → cases will be assigned to groups in week 7

	Measure	Model
Microstructure	week 3	week 5
Viscoelasticity	week 4	week 4
Fracture	week 5	week 6/7

Agenda for today

0. Organization of the module
1. Background and organization of this unit
2. Example of numerical modeling of construction materials
3. Theory and quiz on notations
4. Basics of continuum mechanics

Positioning of this unit

You have had a first introduction in FEM:

- CEGM1000 MUDE
  - Poisson equation
  - Derivation of the method

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This quarter you will see it applied to materials and structures:

- **CIEM1110-1 Numerical modeling of construction materials**
  - Continuum mechanics
  - Diffusion problems
  - Linear and nonlinear FEM
  - Research-oriented software
  - Commercial software
  - Reporting simulation results

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There will be more to learn about numerical modeling:

- CIEM1210-3 Advanced constitutive modeling
  - In-depth about material modeling
- CIEM1301 Advanced computational mechanics
  - Connect to recent literature
- CIEM1303 Upscaling techniques in construction materials design and engineering
  - Focus on multiscale modeling
- Data science and artificial intelligence for engineers (cross-over)
  - Possible application on FEM-AI interface
- CIEM0500 MSc thesis
  - Computer-aided engineering
  - Computational mechanics research

Learning objectives of this unit

After completing this course, you will be able to:

1. Derive the discrete system of equations with the finite element method for continuum elasticity and diffusion problems
2. Explain the concepts of the nonlinear finite element method and its use for material and structural analysis
3. Select an appropriate mathematical model that idealizes the physical problem of analysis of a material characterization test (field equation, boundary conditions, material model)
4. Perform and evaluate nonlinear finite element simulations of material characterization tests
5. Apply discrete (lattice) models for fracture and transport problems in view of durability of materials
6. Report the results from computational analysis of material behaviour also conveying the uncertainty in these results

Organization of this unit

Three weekly slots for **contact hours**

- Monday 15:45-17:30, 3.02
- Wednesday 13:45-15:30, Echo-D
- Thursday 15:45-17:30, 1.21

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Rough **overview** of the content (and instructors)

- Weeks 1–4: FEM formulation and implementation (Frans van der Meer, Martin Lesueur, Iuri Rocha, Cor Kasbergen)
- Week 5: Lattice modeling (Branko Šavija)
- Weeks 6-8: Applied FEM (Rita Esposito)

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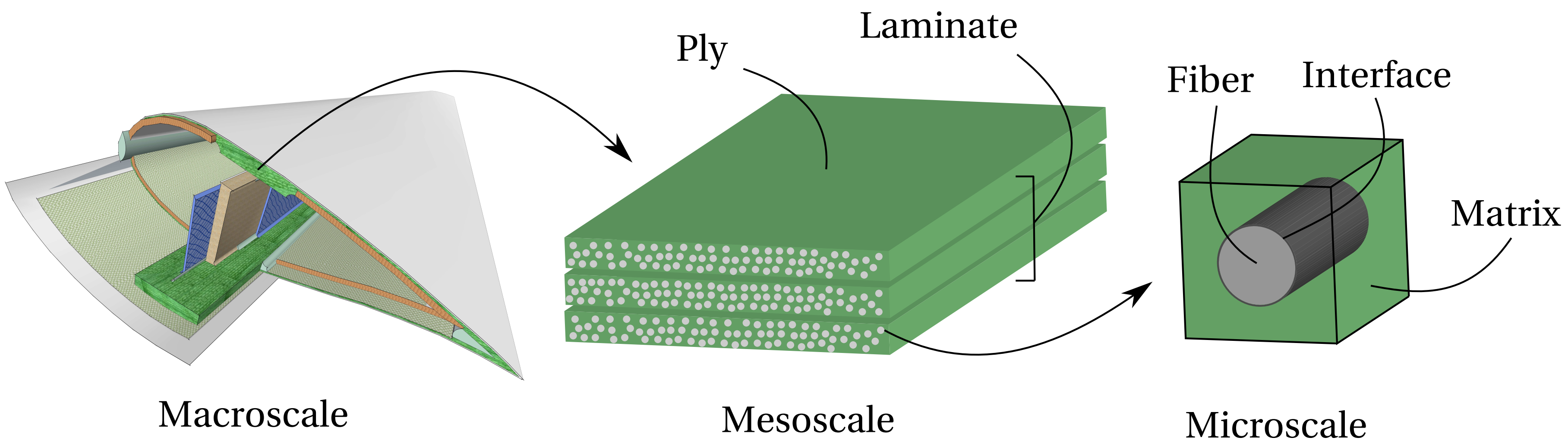
Activities for this week

- This lecture: Example of scientific numerical modeling of materials, notations, continuum mechanics
- Self study: Introduction chapter from jupyter book
- Wednesday: Introduction into `pyJive`
- Thursday: Interactive lecture including review of MUDE material

Many engineering challenges require advanced material modeling

An example: hygrothermal aging of fiber-reinforced polymers

- **Goal:** make wind turbine blades last longer by reducing material behavior uncertainties
- **Experimental observation:** the material loses half of its strength after exposure to hot water



Rocha et al. (2017)–(2019)

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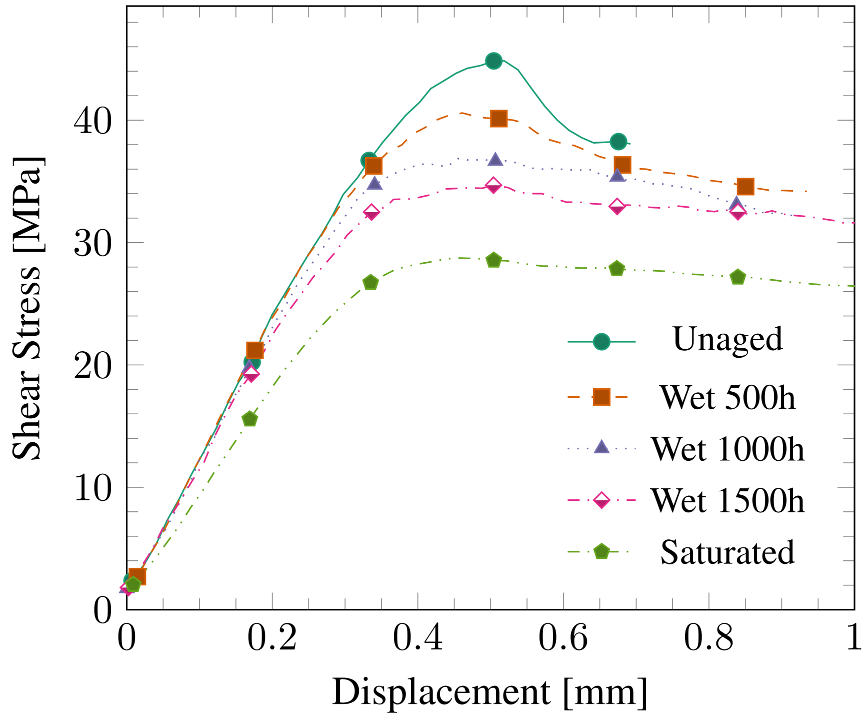
aging

testing

processing



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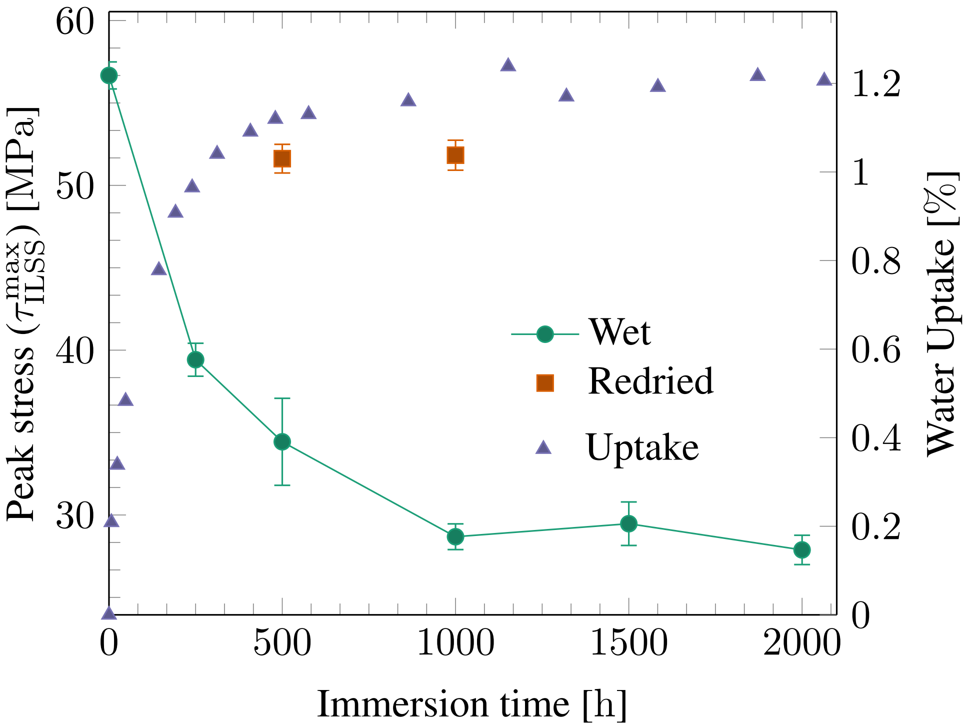
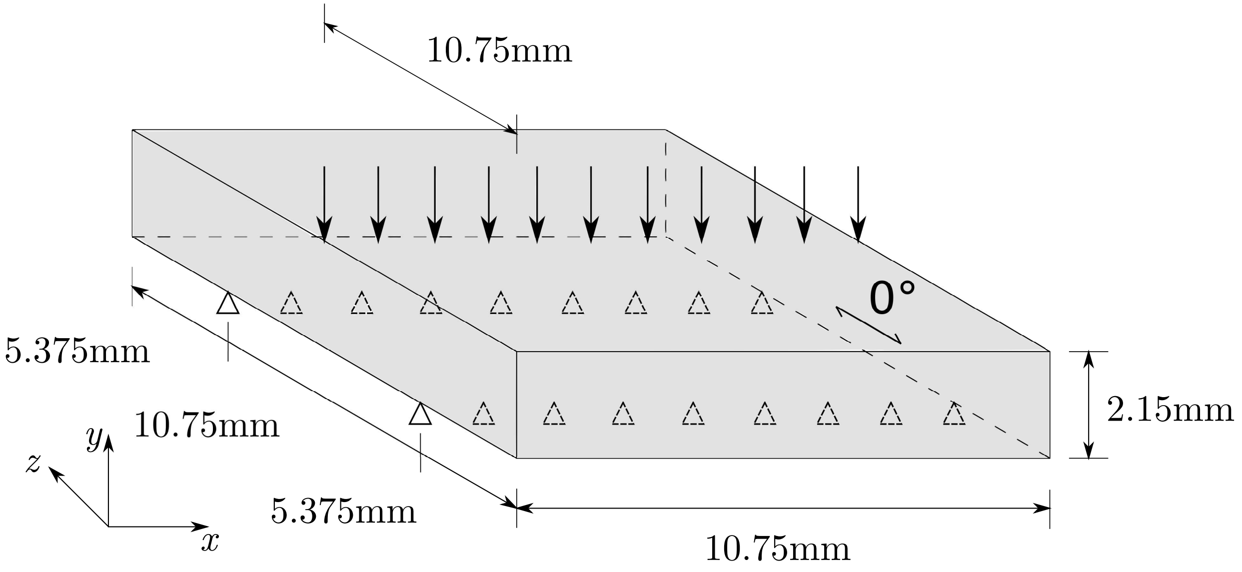
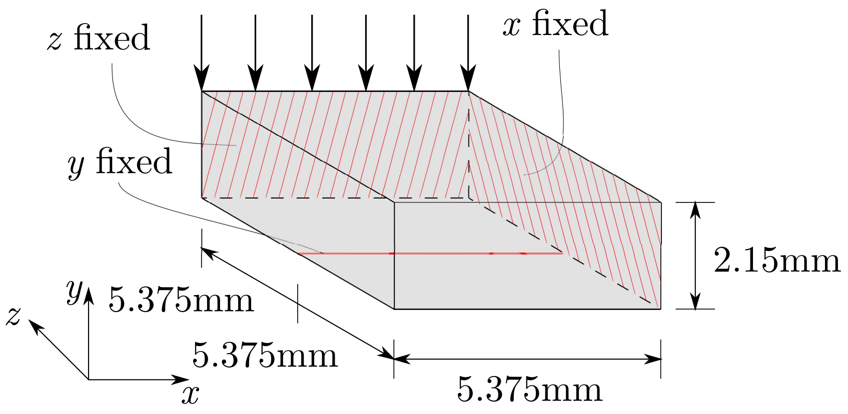


Using FEM to tackle the problem

- Symmetry is exploited in order to reduce computational effort





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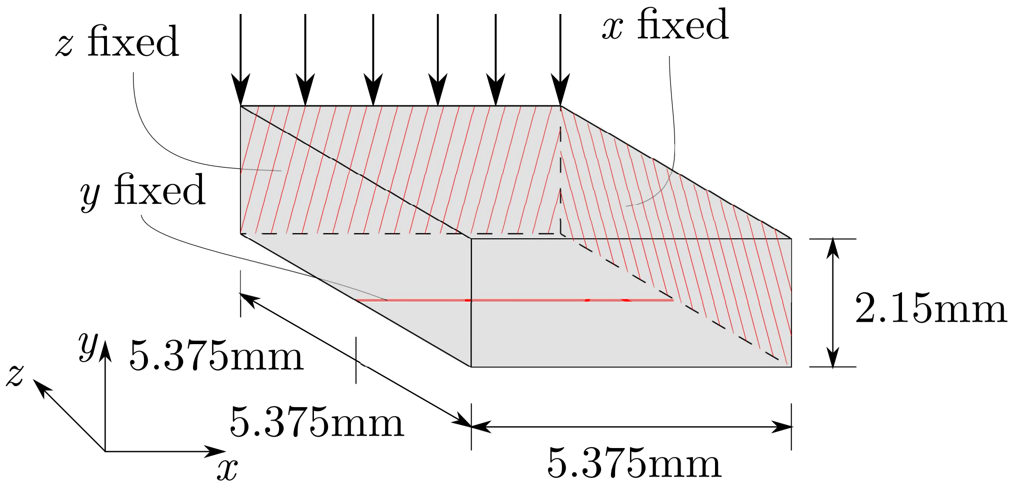
- Symmetry is exploited in order to reduce computational effort
- Three-dimensional 8-node elements used to simulate mechanical equilibrium



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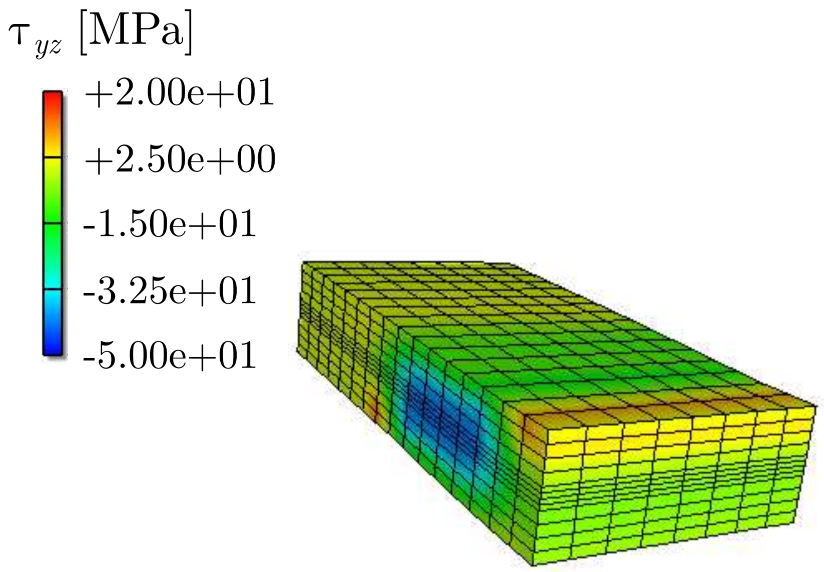
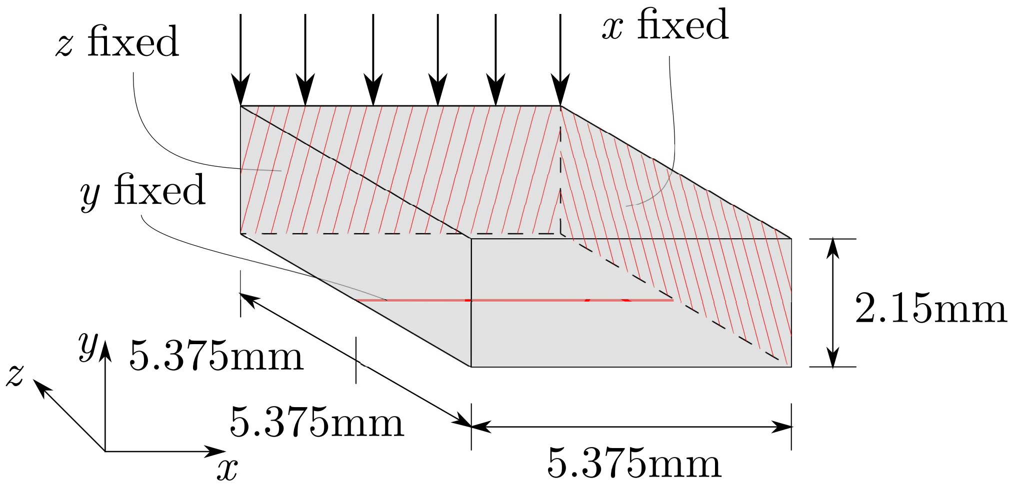


Using FEM to tackle the problem

- Symmetry is exploited in order to reduce computational effort
- Three-dimensional 8-node elements used to simulate mechanical equilibrium
- What is the material behavior?



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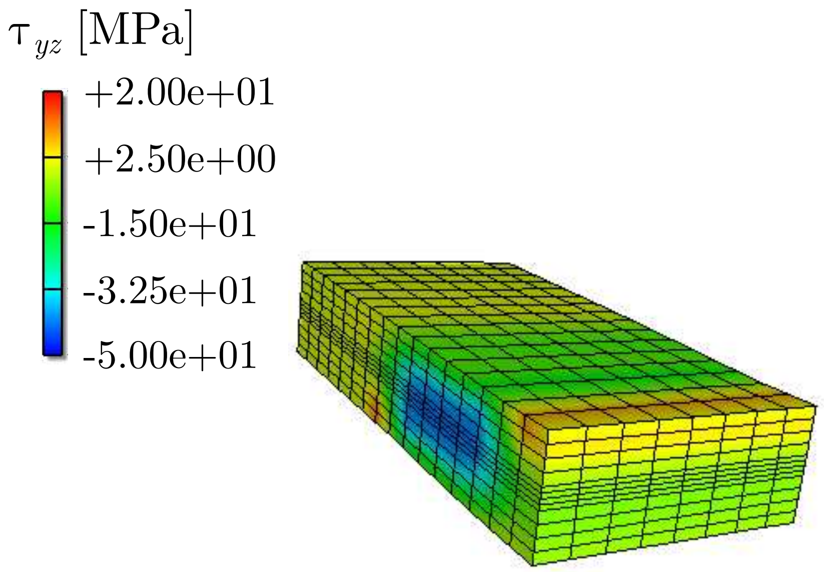
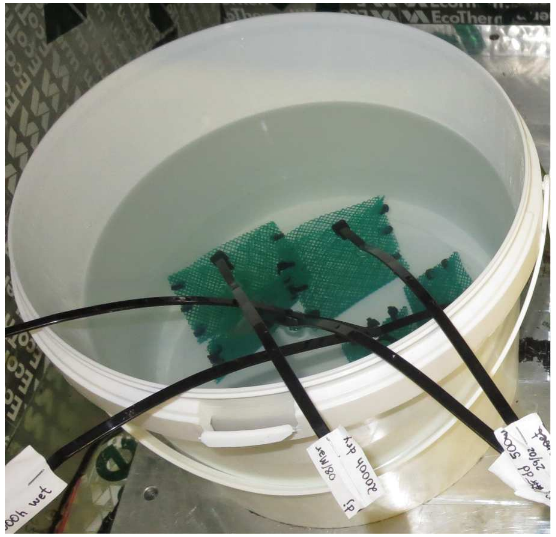


Adding another layer of FEM to the simulation

Mechanical equilibrium does not tell the whole story. Aging is driven by water ingression



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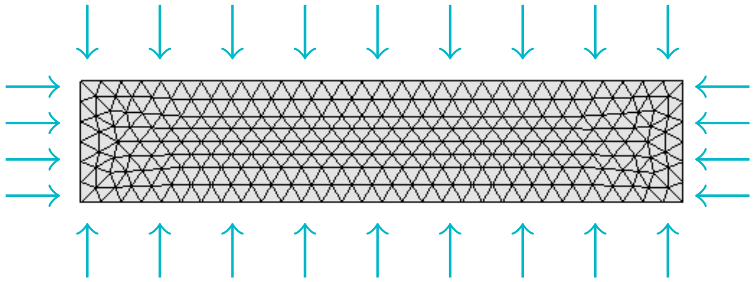

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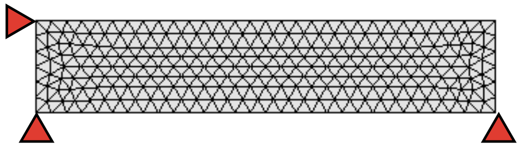

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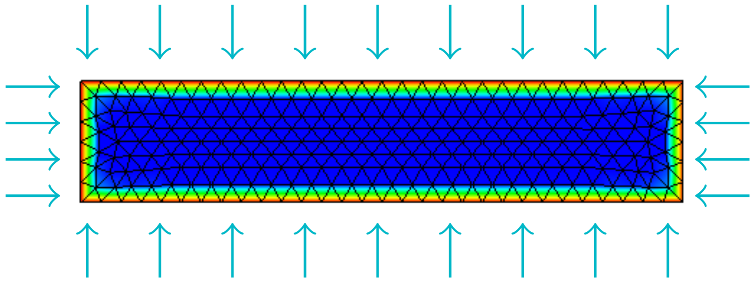

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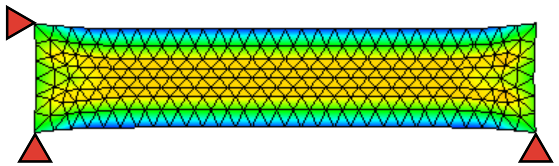

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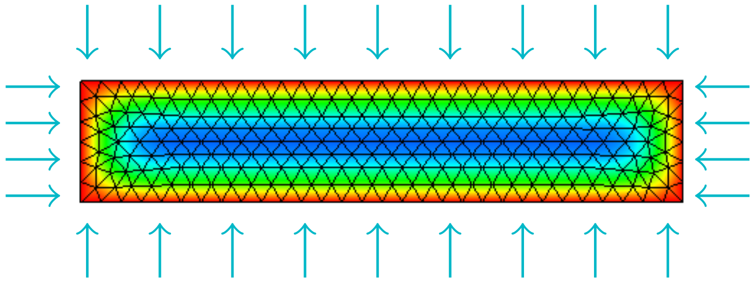

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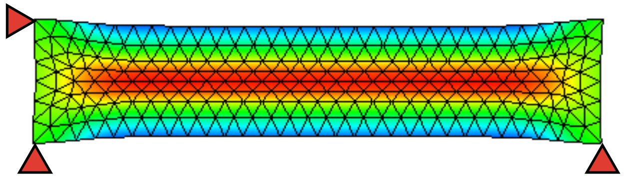

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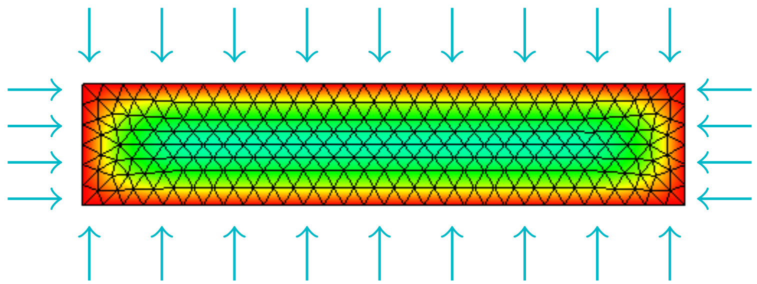

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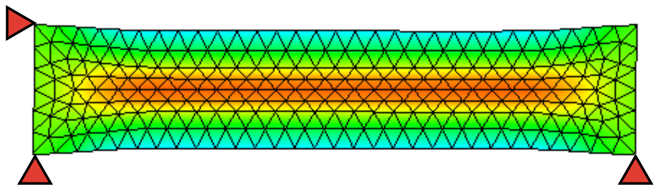

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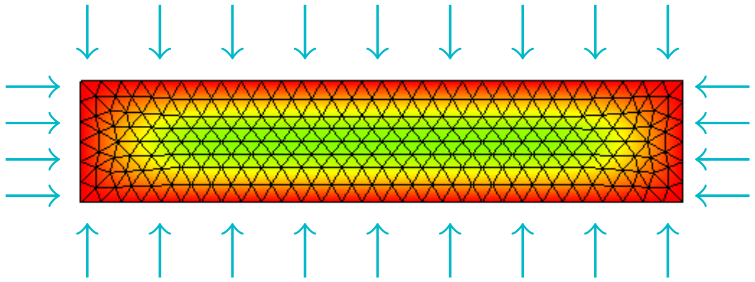

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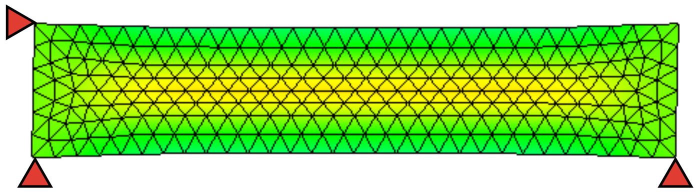

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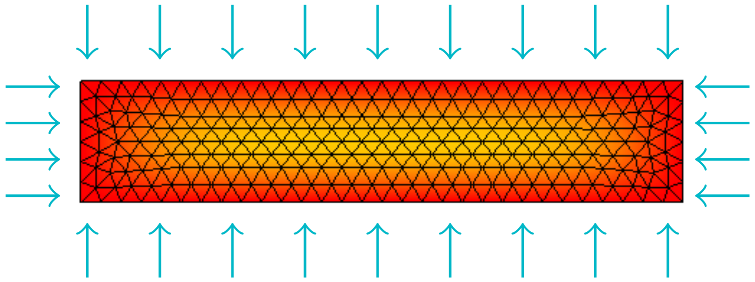

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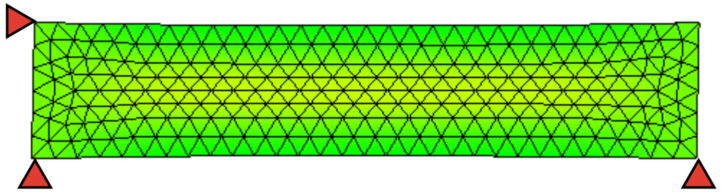

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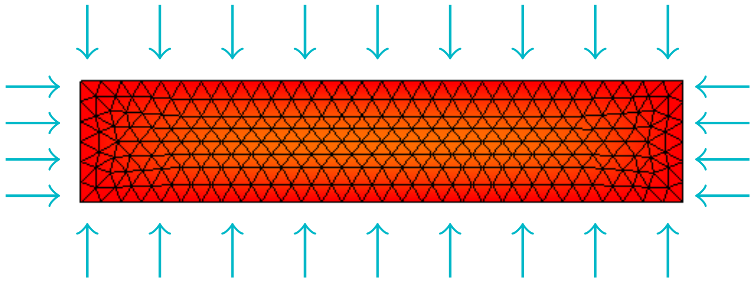

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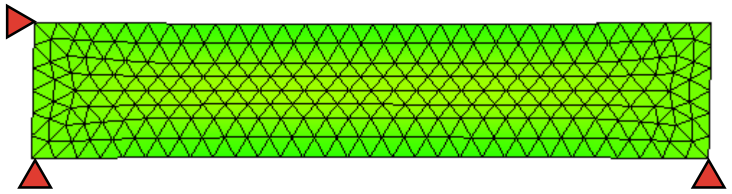

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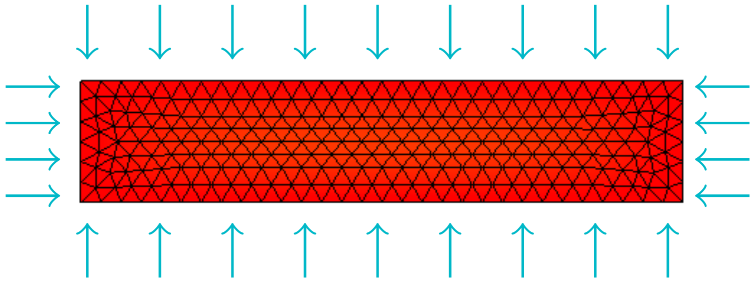

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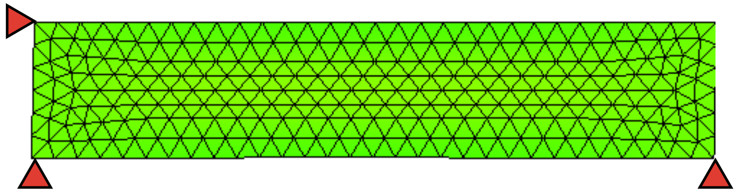
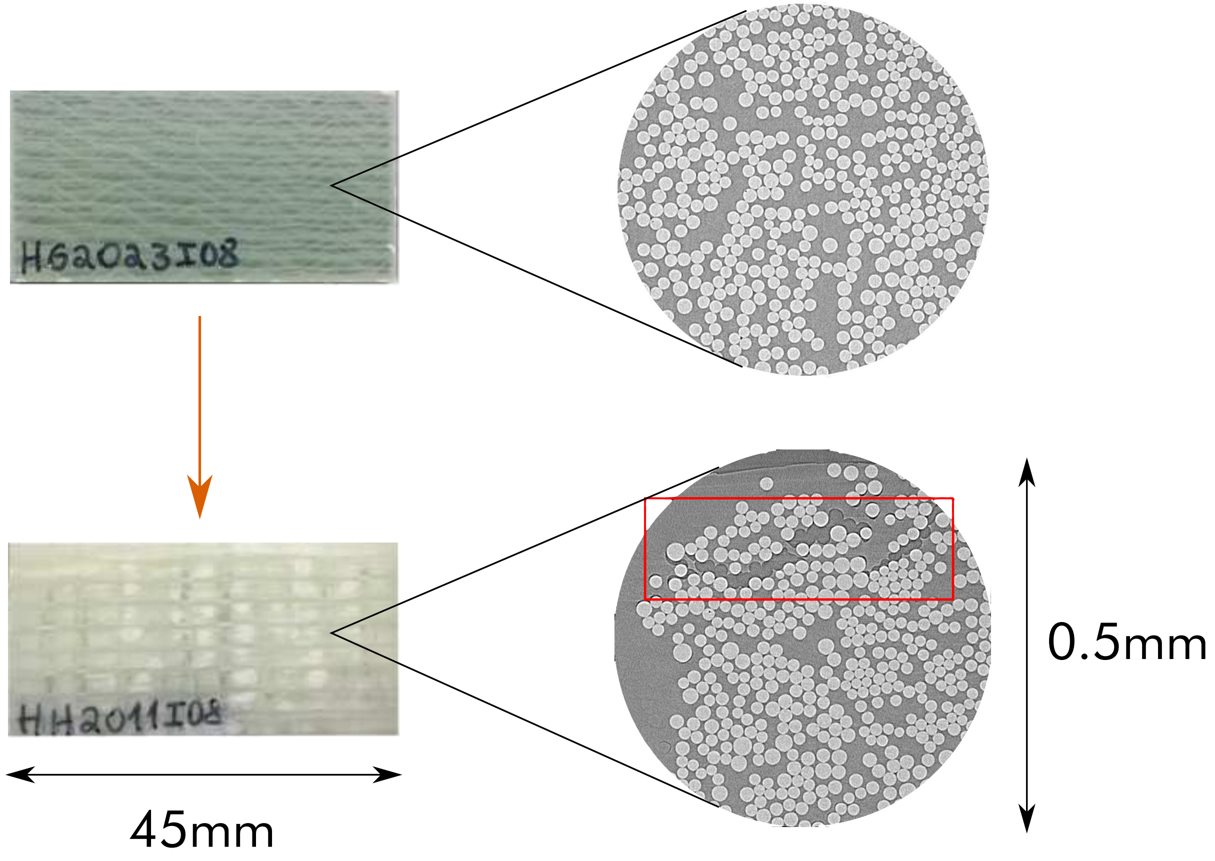


Adding FEM models on a different spatial scale

But that is still not enough. Hygrothermal aging is a multiscale problem



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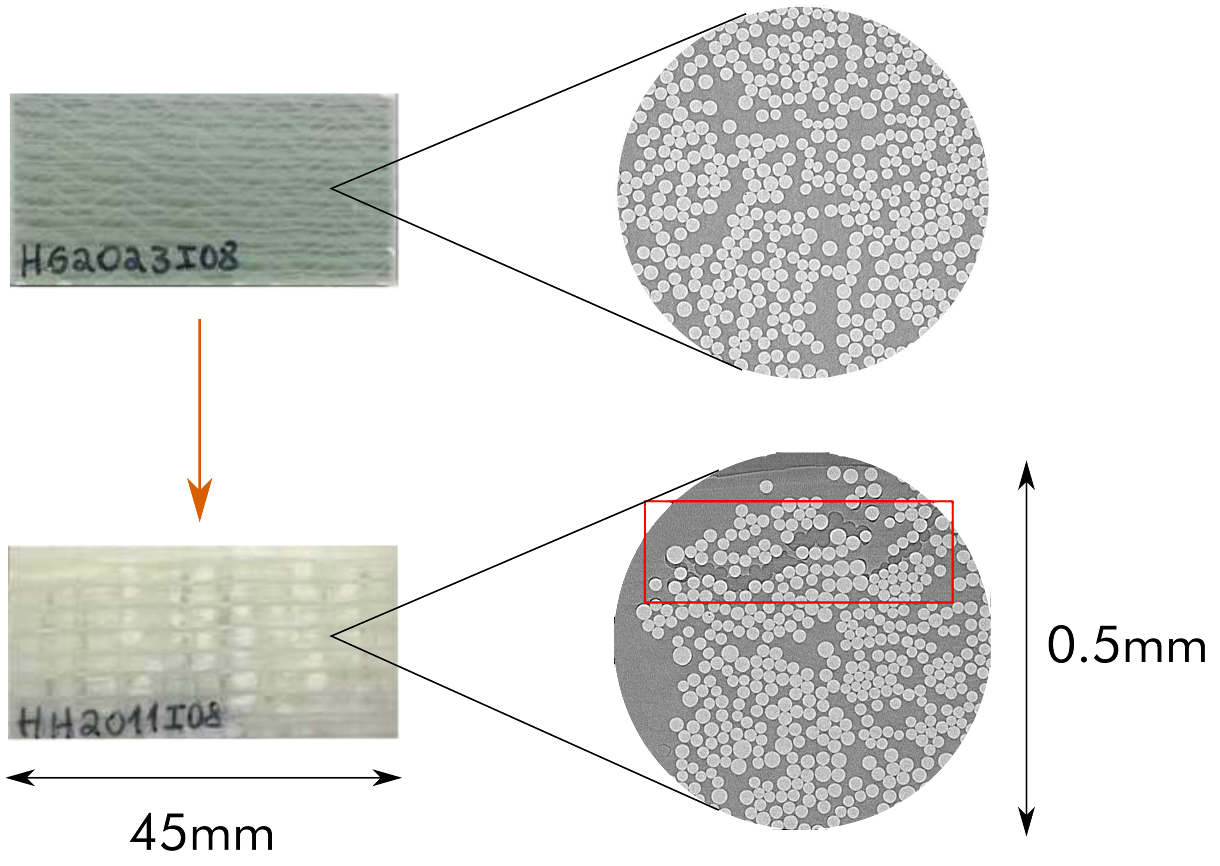

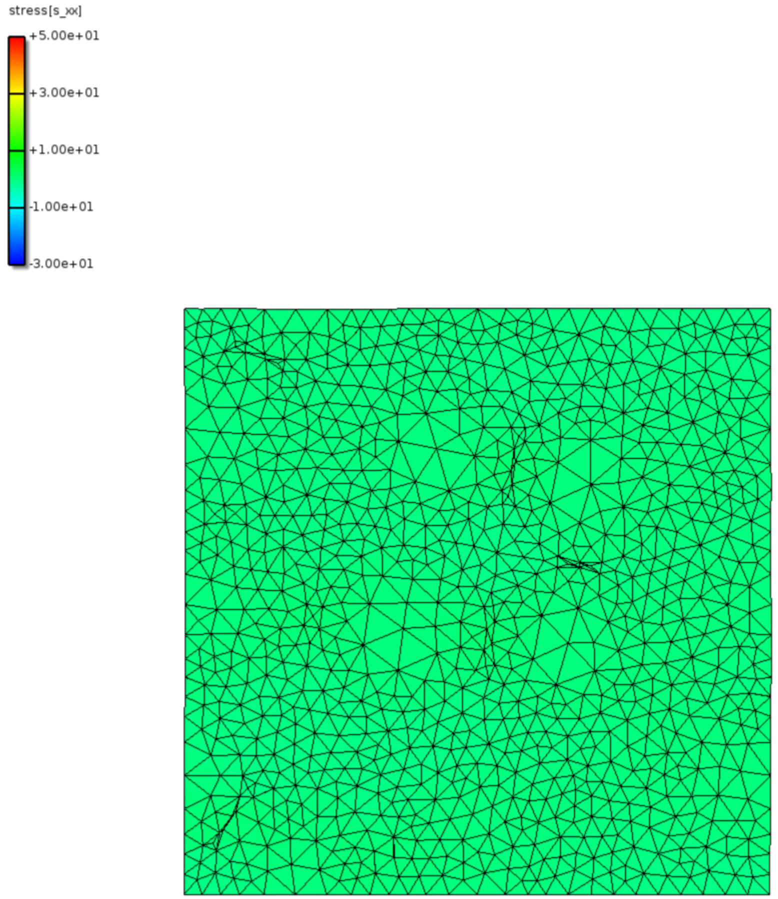

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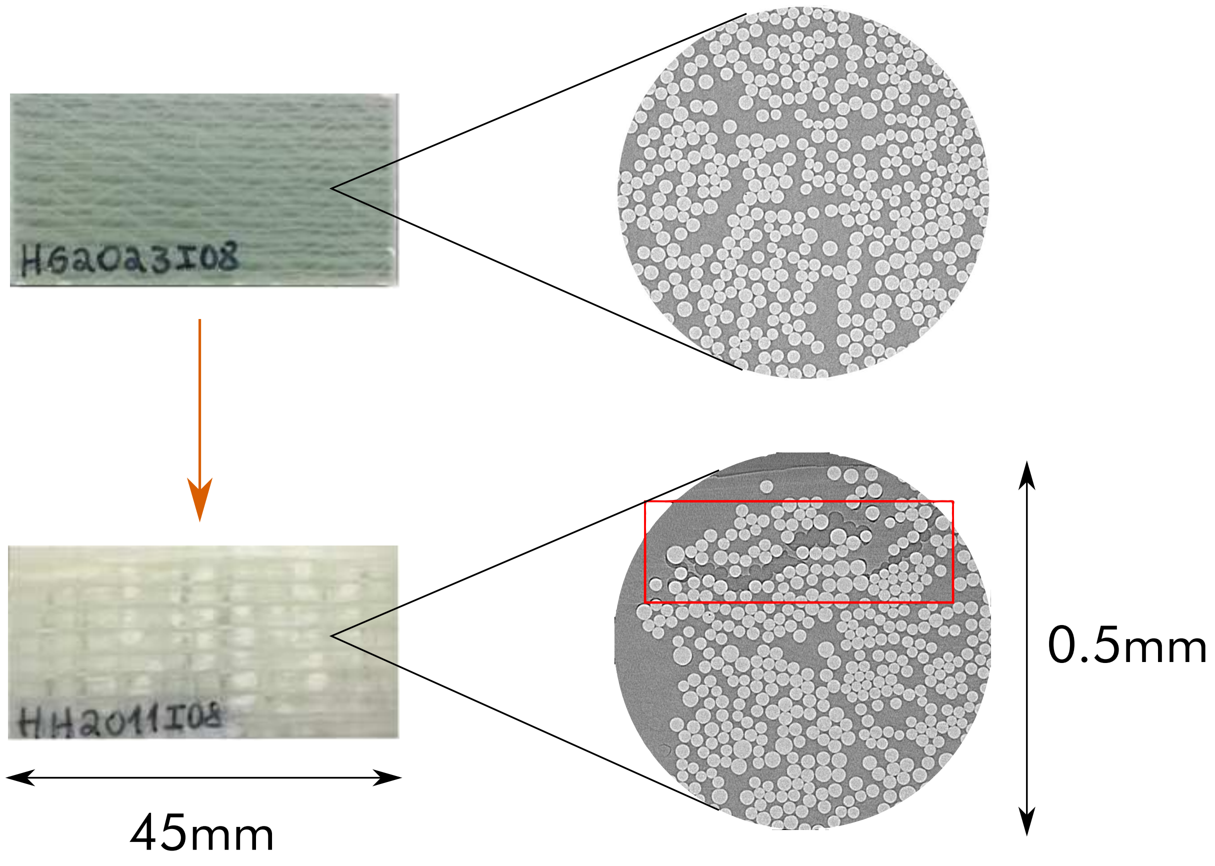

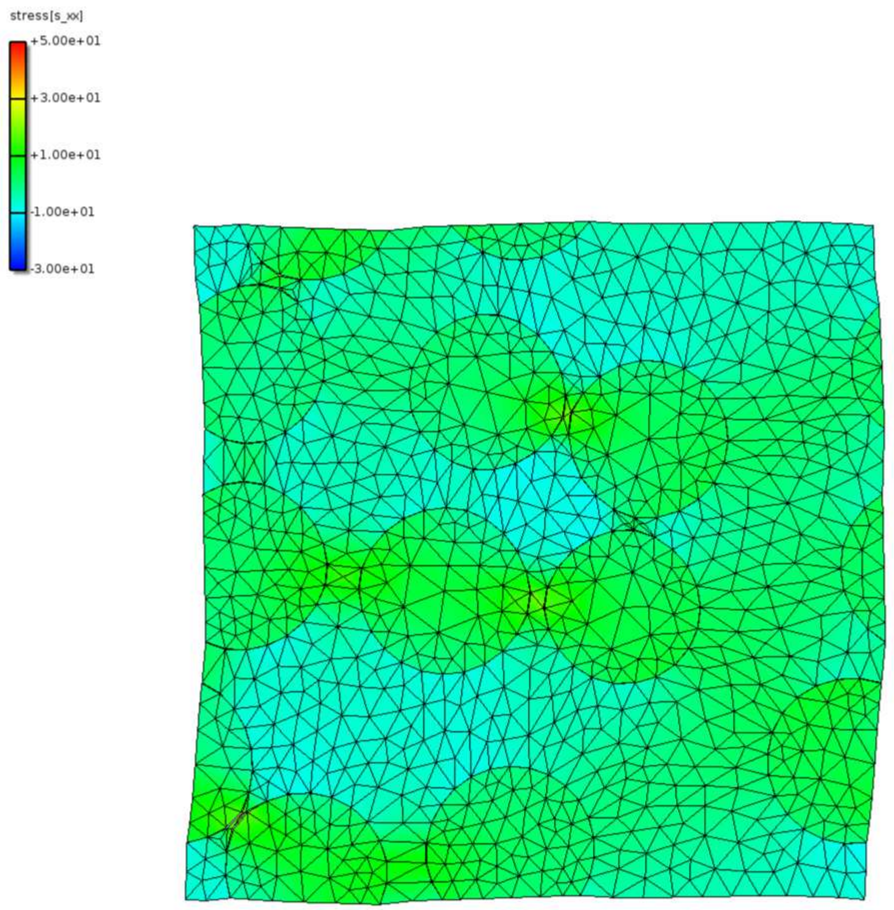

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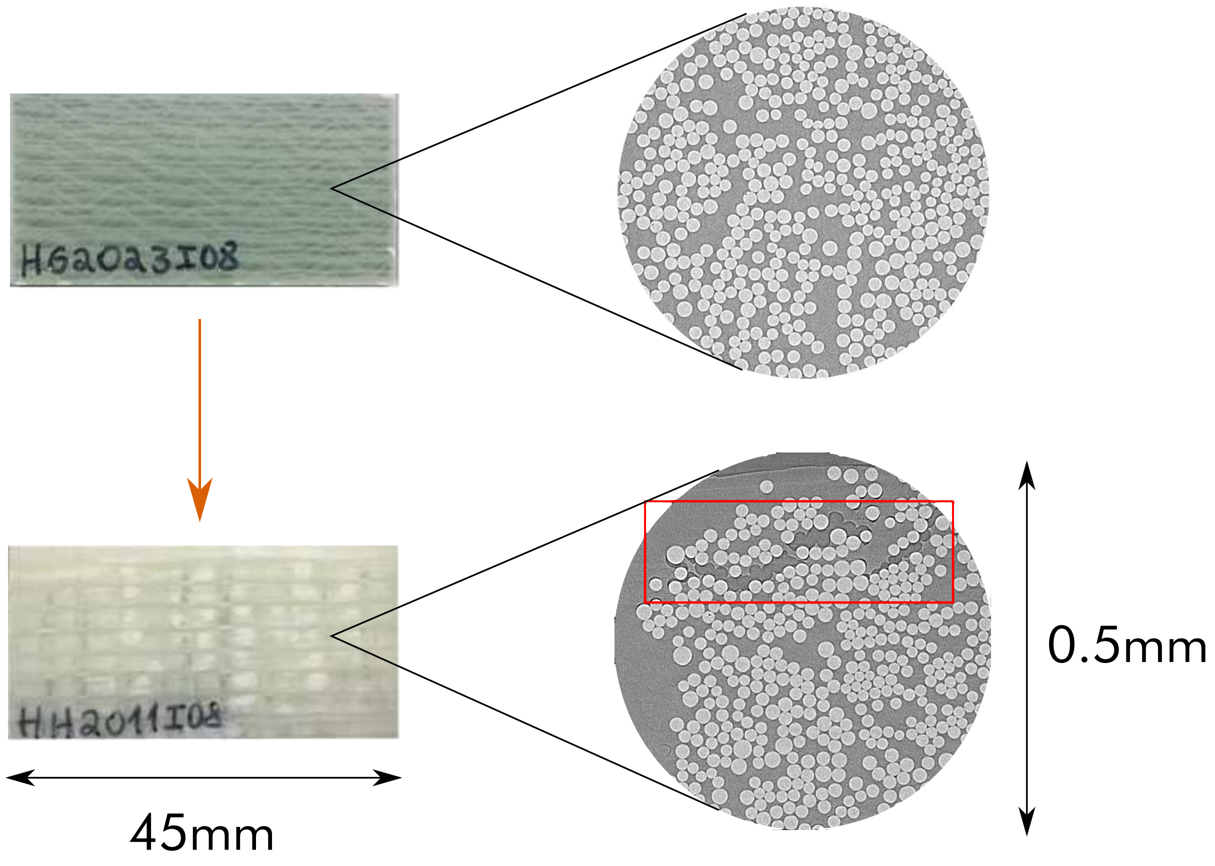

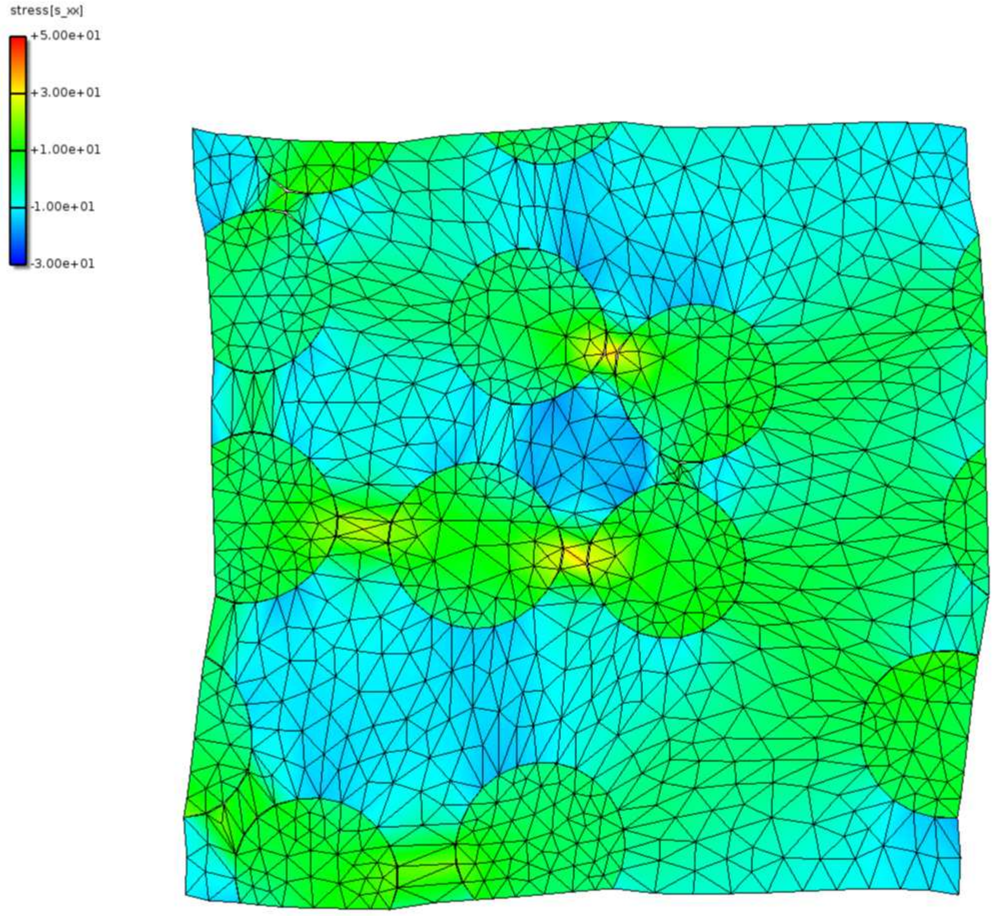

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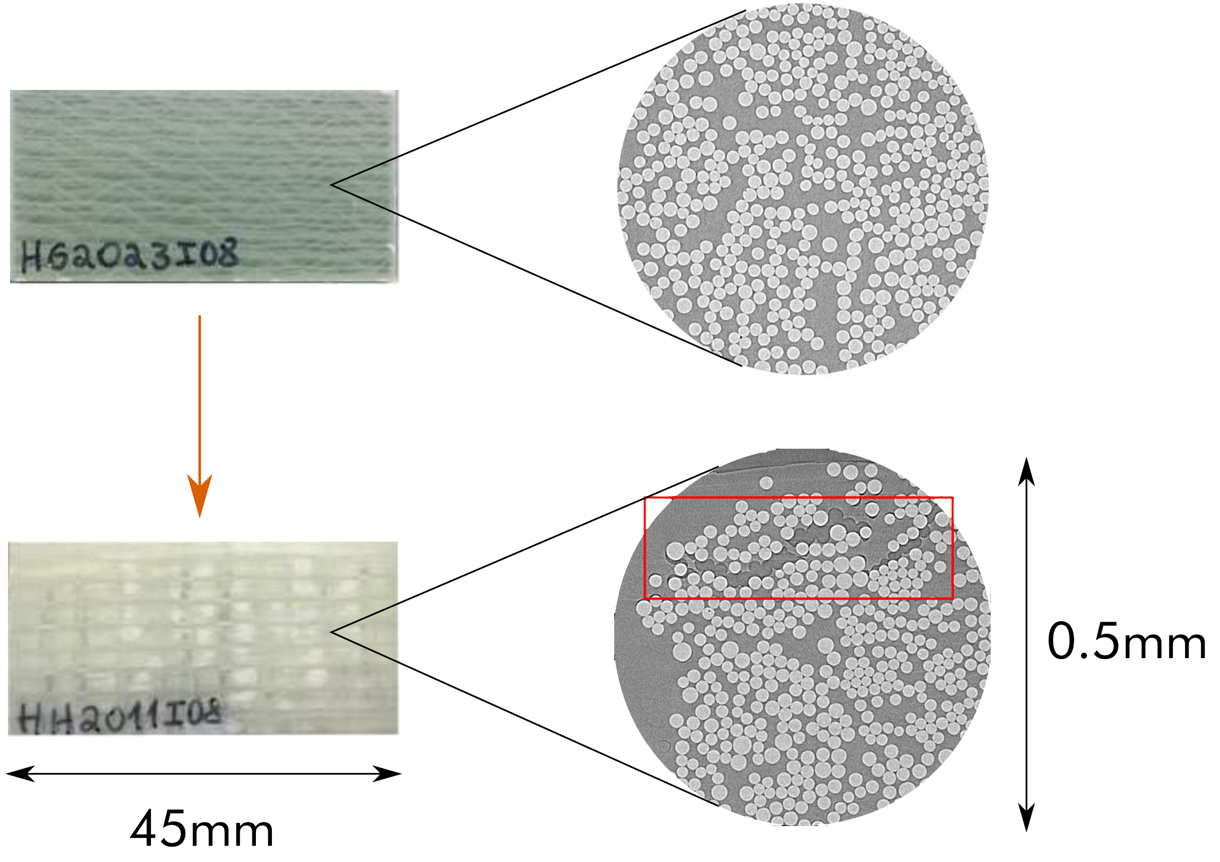

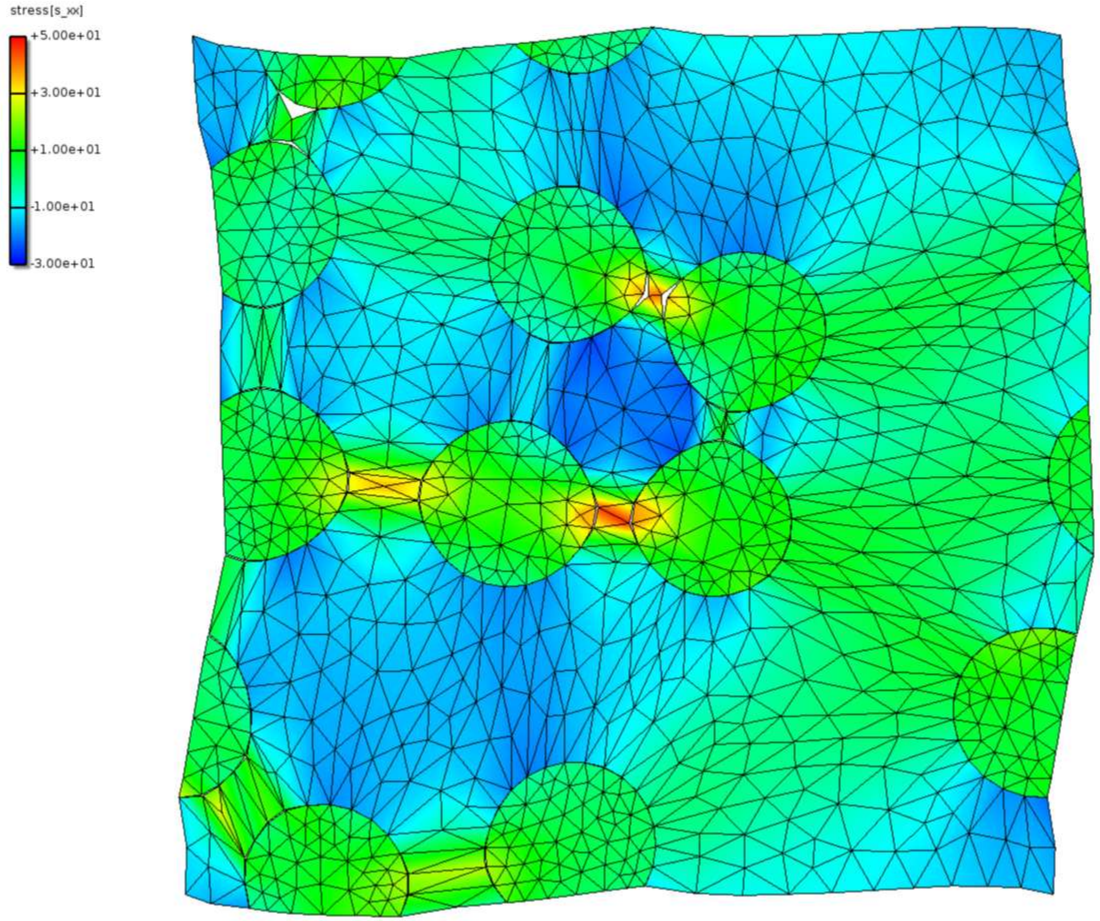

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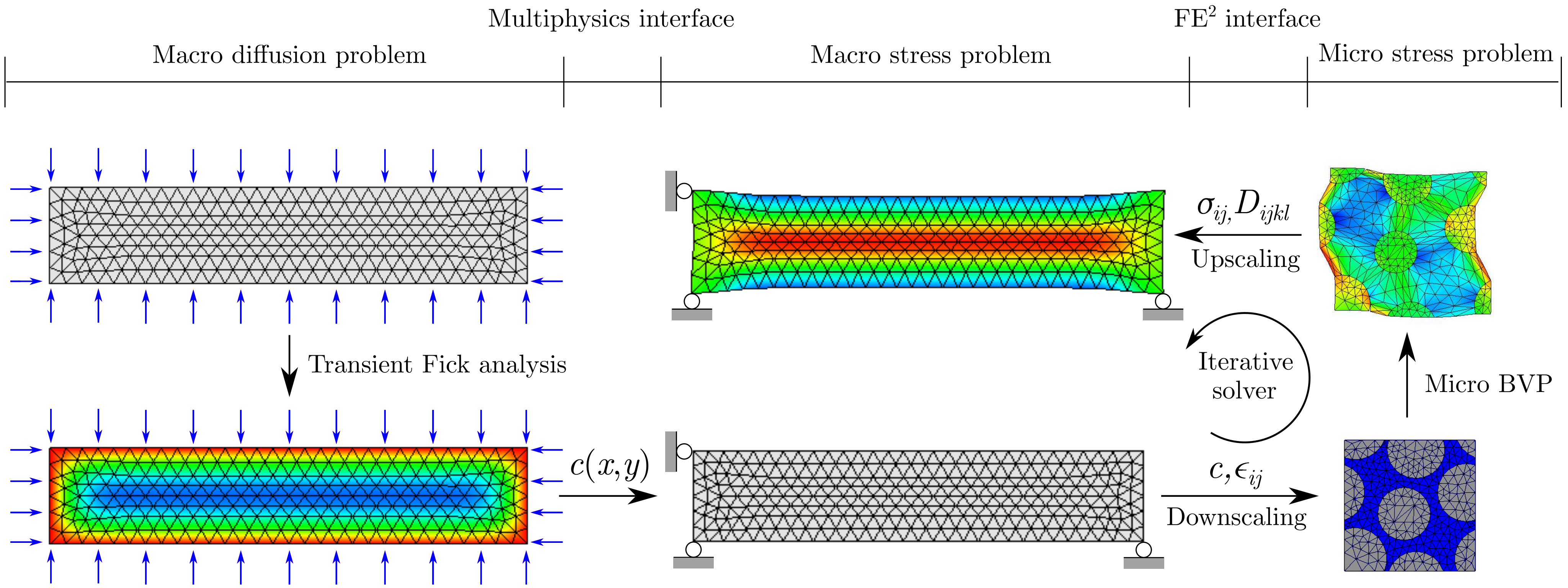
Bringing different scales and physical quantities together

- **Macroscale:** FEM for water diffusion + FEM for mechanical equilibrium
- **Microscale:** FEM for mechanical equilibrium with fixed water concentration



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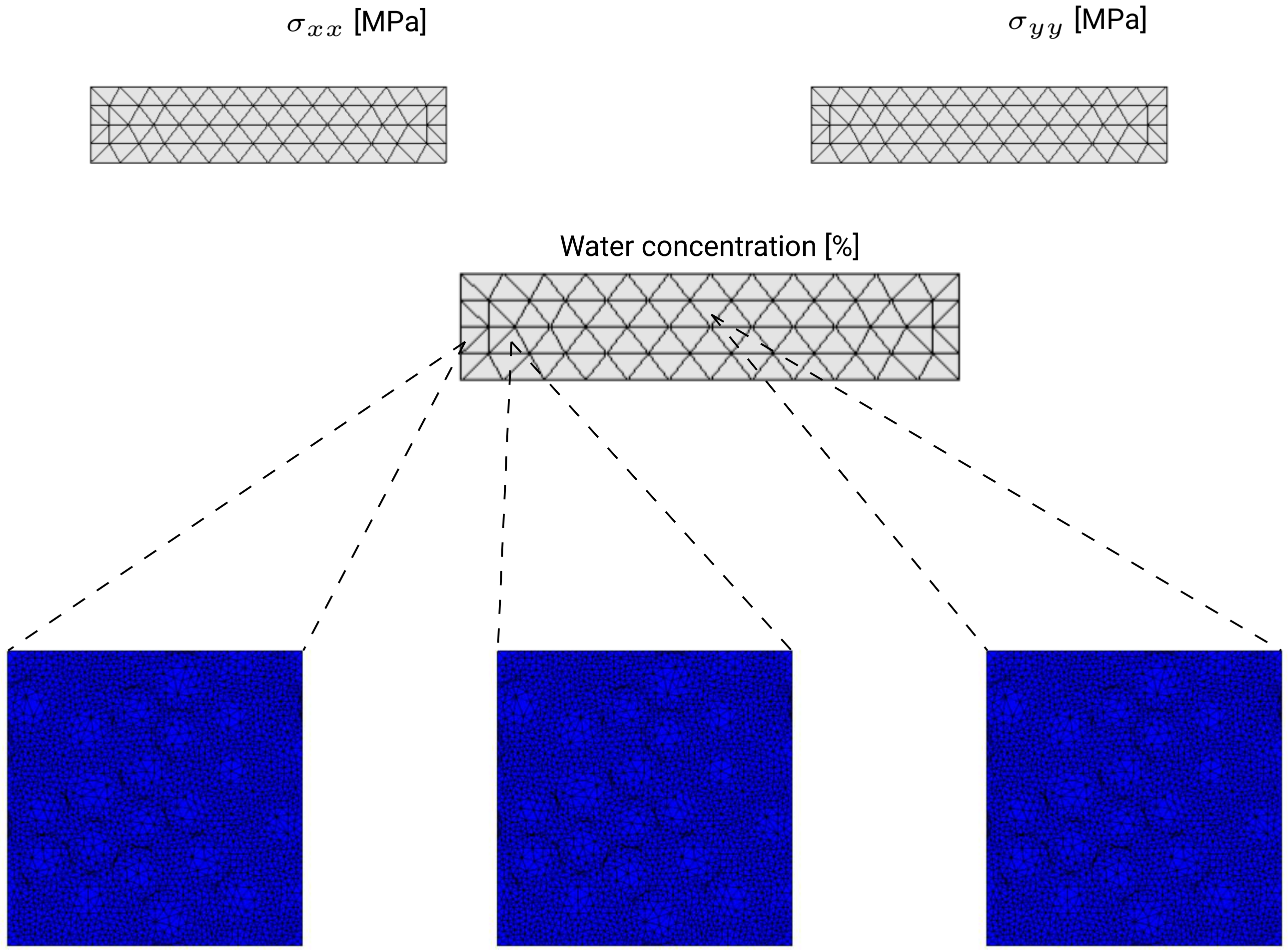

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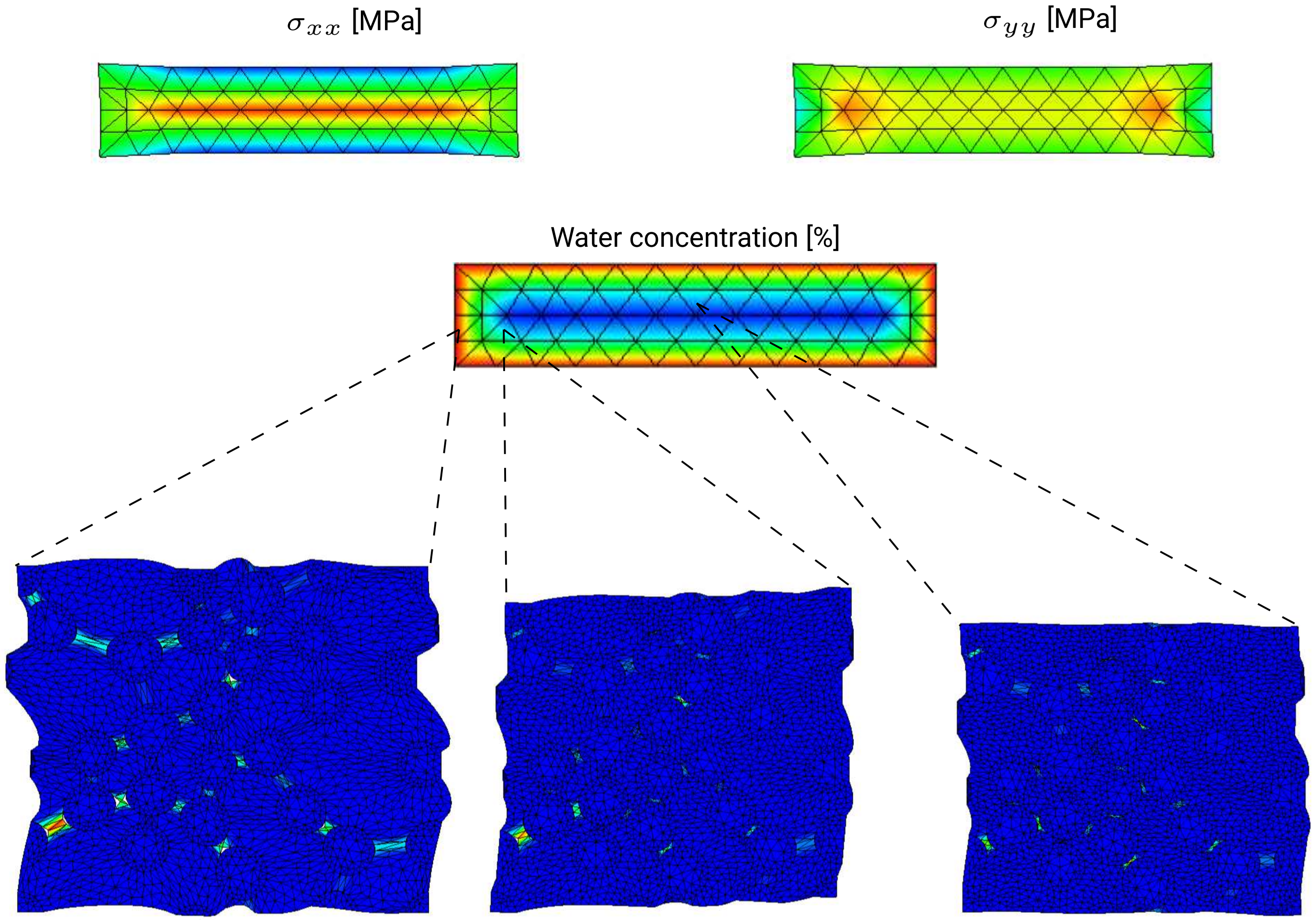

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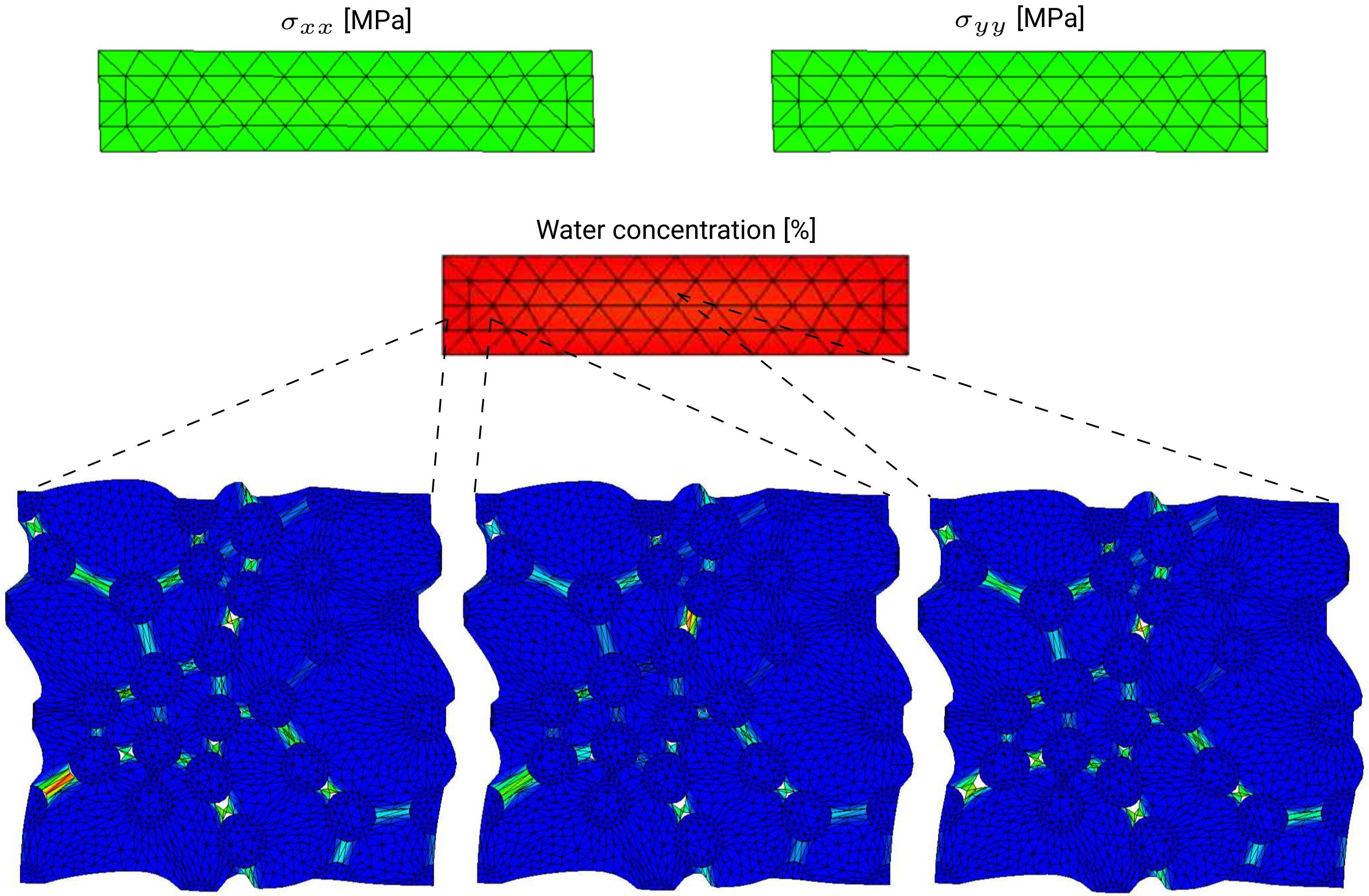

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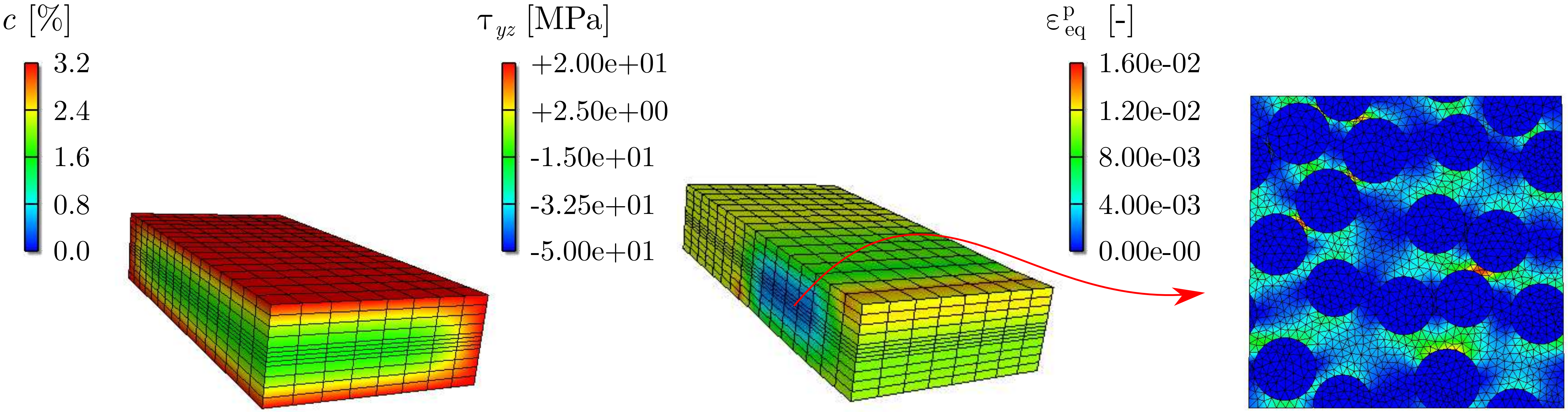
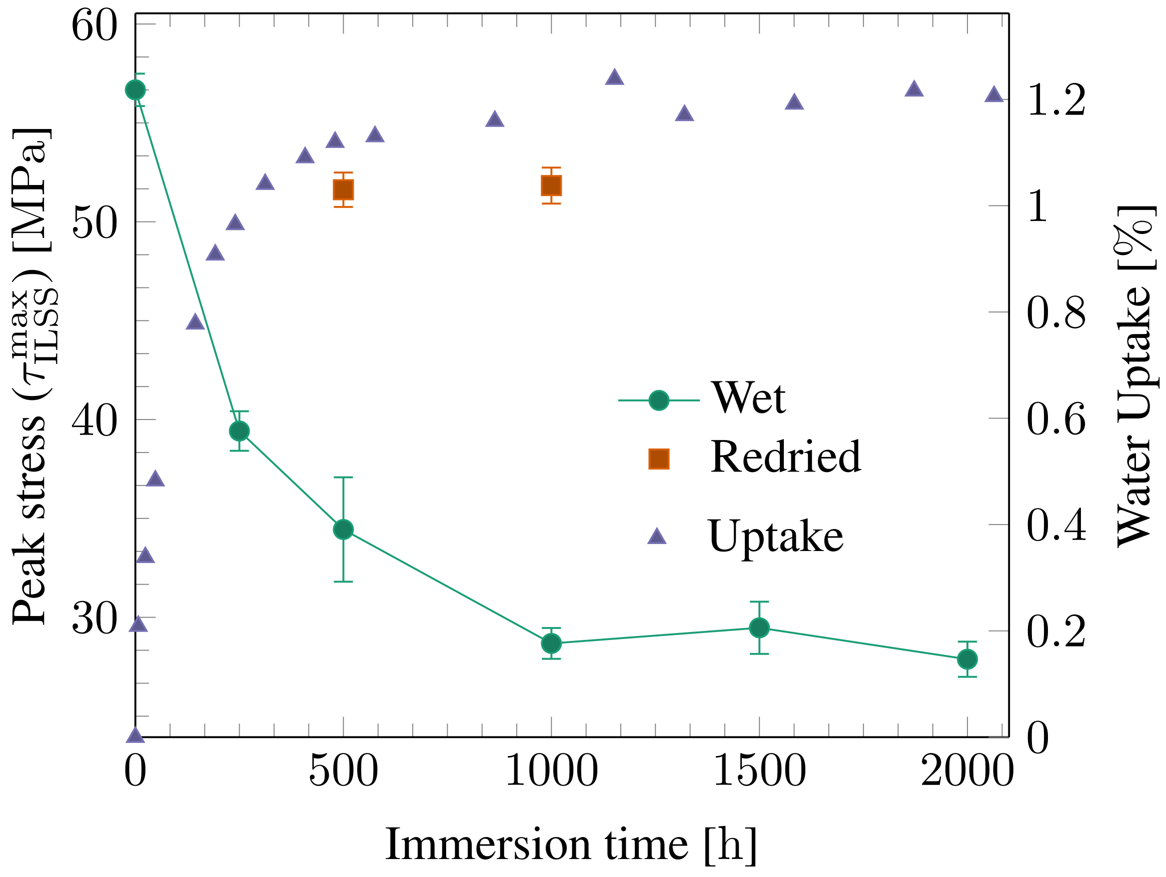
Performing virtual test on partially saturated specimen

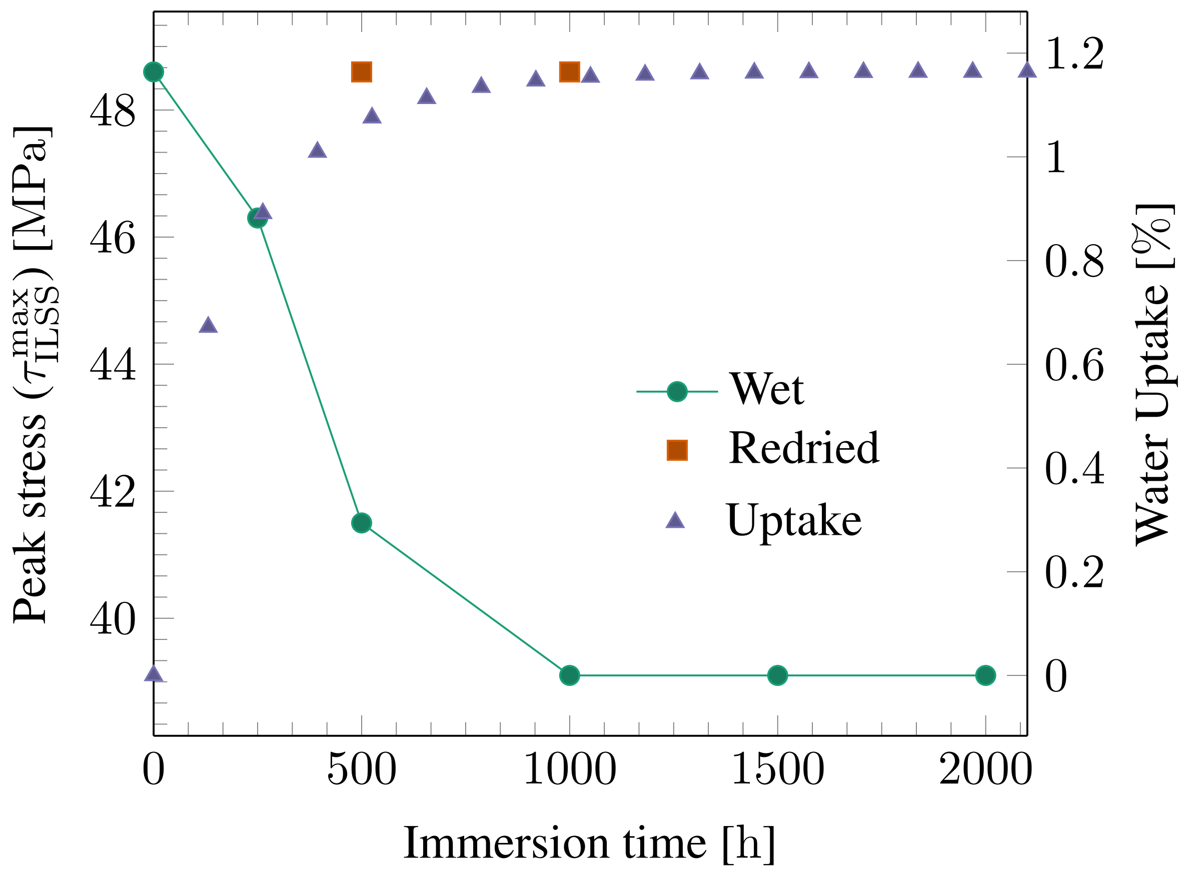


Reproducing experimental observations and beyond

Experimental observations



Numerical results



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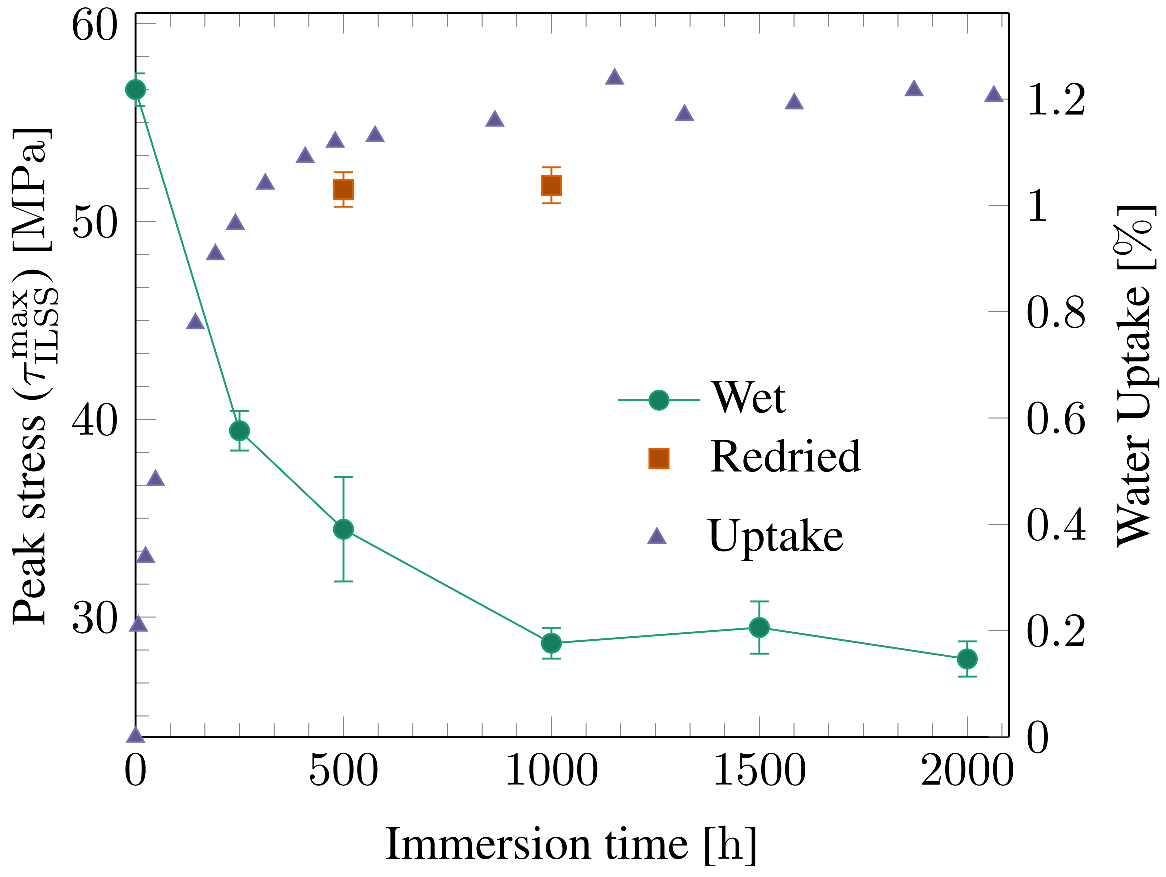
Experimental observations



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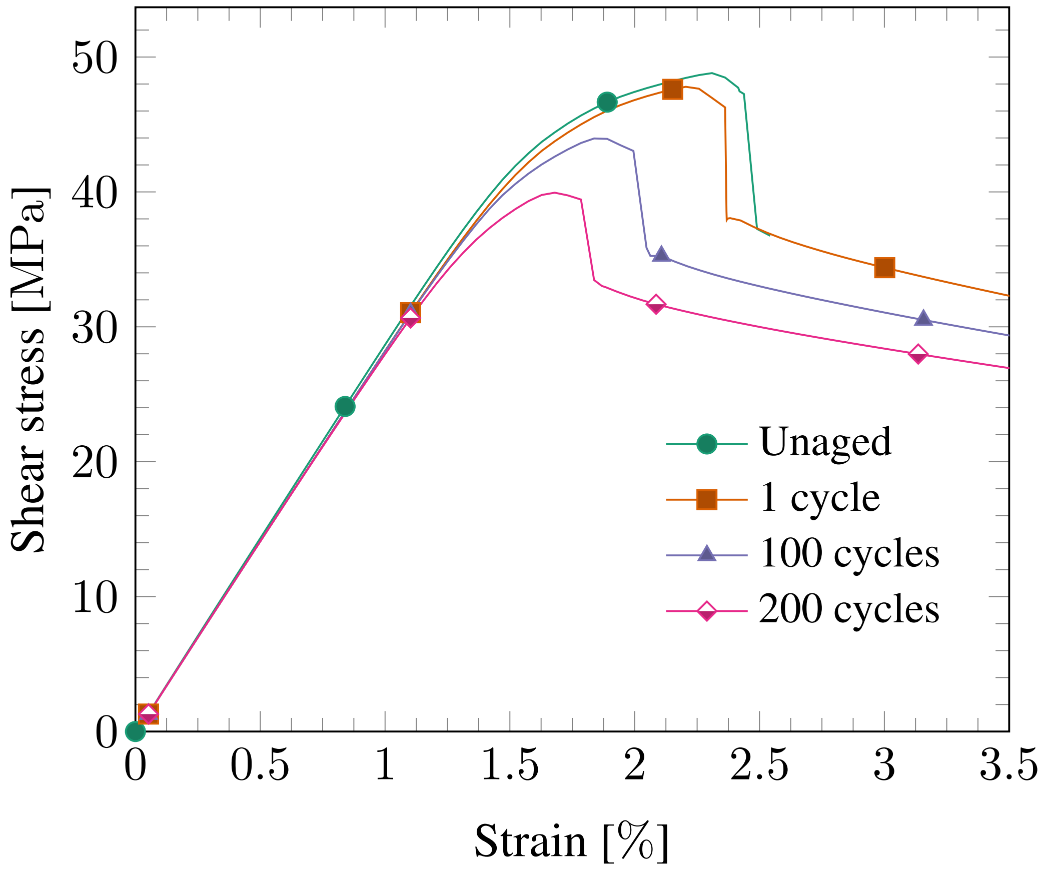

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Takeaways from this example

How is this related to what you will learn in this unit:

- Models are crucial in understanding material behavior
- The finite element method can be used to model various physical processes
- The most relevant ones are mechanical equilibrium and transport
- The finite element method is very suitable for complex geometries (including microstructures)
- Many relevant problems are nonlinear

Tensors in different notations

	Tensor notation	Components	Index notation
Scalar (zero order tensor)	a	a	a
Vector (first order tensor)	$\mathbf{a}$	$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}$	a_i
Matrix (second order tensor)	$\mathbf{A}$	$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix}$	A_{ij}
Fourth order tensor	$\boldsymbol{\mathcal{A}}$	-	$\mathcal{A}_{ijkl}$

Multiplication in different notations

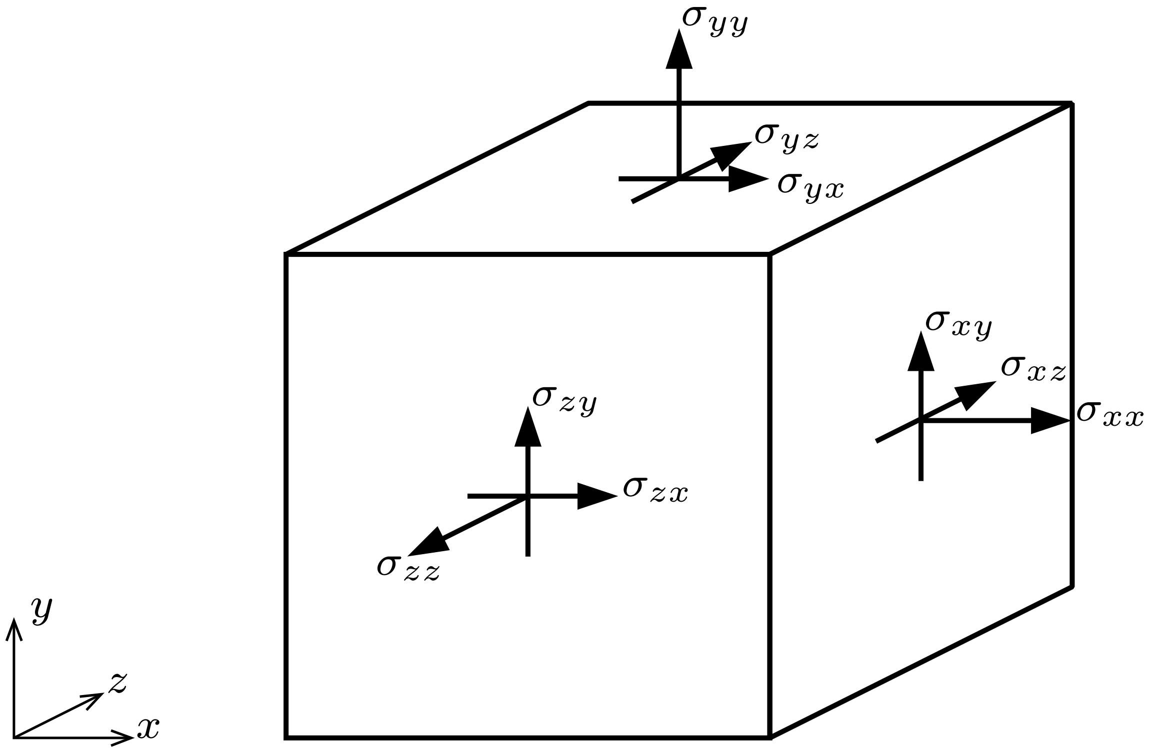
	Matrix/vector notation	Tensor notation	Index notation
Matrix-vector product	$\mathbf{A}\mathbf{b}$	$\mathbf{A} \cdot \mathbf{b}$	$A_{ij} b_j$
Dot product	$\mathbf{a}^T \mathbf{b}$	$\mathbf{a} \cdot \mathbf{b}$	$a_i b_i$
Tensor product	$\mathbf{a}\mathbf{b}^T$	$\mathbf{a} \otimes \mathbf{b}$	$a_i b_j$
Double dot product	-	$\mathbf{A} : \mathbf{B}$	$A_{ij} B_{ij}$
Double dot product	-	$\boldsymbol{\mathcal{C}} : \mathbf{A}$	$\mathcal{C}_{ijkl} A_{kl}$
Matrix-matrix product	$\mathbf{A}\mathbf{B}$	$\mathbf{A} \cdot \mathbf{B}$	$A_{ik} B_{kj}$
Matrix-matrix with a transpose	$\mathbf{A}^T \mathbf{B}$	$\mathbf{A}^T \cdot \mathbf{B}$	$A_{ki} B_{kj}$
Cross product	$\mathbf{a} \times \mathbf{b}$	$\mathbf{a} \times \mathbf{b}$	$\epsilon_{ijk} a_j b_k$

Exercise

Test yourself with brightspace quiz *Notations and products*

Continuum mechanics: stress and strain

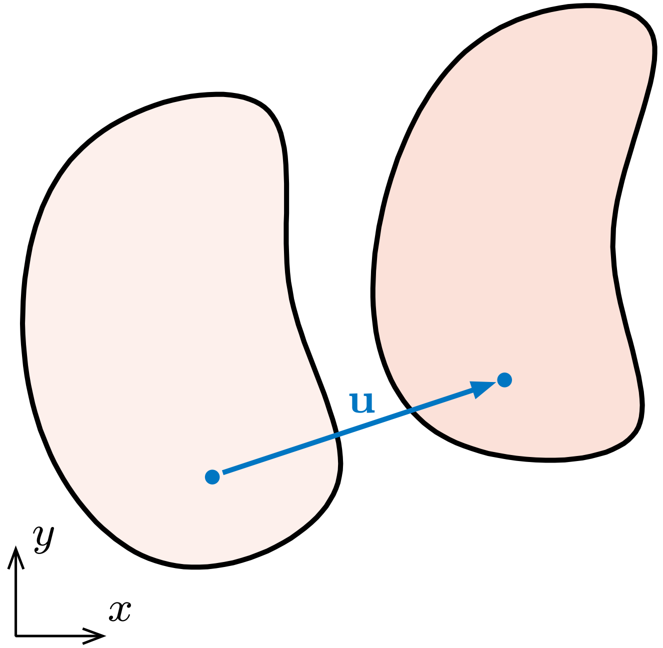
Stress tensor on elementary cube



Stress relates traction $\mathbf{t}$ to normal $\mathbf{n}$

$$\mathbf{t} = \boldsymbol{\sigma}\mathbf{n}$$

Displacement is a vector

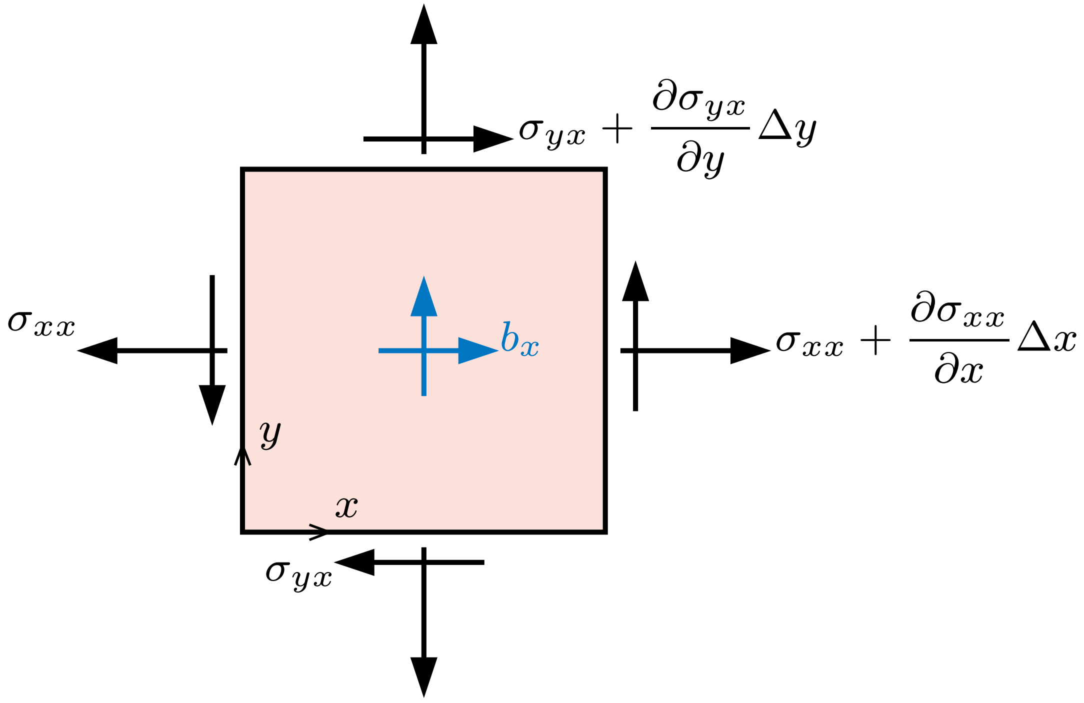


And strain its symmetric gradient

$$\boldsymbol{\varepsilon} = \nabla_s \mathbf{u} = \frac{1}{2}\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right)$$

Continuum mechanics: equilibrium

Translational equilibrium (linear momentum):

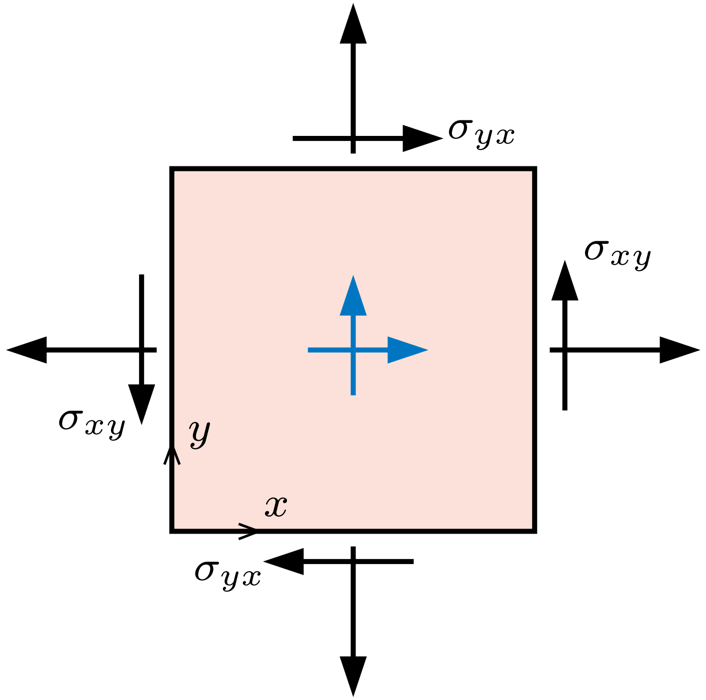


$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} + b_x = 0 \quad \text{etc}$$

or

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{b} = 0$$

Rotational equilibrium (angular momentum):



$$\sigma_{xy} = \sigma_{yx}, \quad \text{etc}$$

or

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$$

Continuum mechanics: linear elasticity

Stress is related to strain through a fourth order tensor

$$\boldsymbol{\sigma} = \mathcal{D} : \boldsymbol{\varepsilon} \quad \text{or} \quad \sigma_{ij} = D_{ijkl}\varepsilon_{kl}$$

In Voigt notation (with stress and strain as vectors) this can be written out, most conveniently in compliance format (relating strain to stress)

$$\begin{Bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \gamma_{yz} \\ \gamma_{zx} \\ \gamma_{xy} \end{Bmatrix} = \frac{1}{E} \begin{bmatrix} 1 & -\nu & -\nu & 0 & 0 & 0 \\ -\nu & 1 & -\nu & 0 & 0 & 0 \\ -\nu & -\nu & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2+2\nu & 0 & 0 \\ 0 & 0 & 0 & 0 & 2+2\nu & 0 \\ 0 & 0 & 0 & 0 & 0 & 2+2\nu \end{bmatrix} \begin{Bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \end{Bmatrix}$$

Continuum mechanics: 2D

There are three different ways to go from 3D to 2D:

- Plane stress ($\sigma_{zz} = 0$)
- Plane strain ($\epsilon_{zz} = 0$)
- Axisymmetry (starting from (r, z, θ) instead of (x, y, z), $\epsilon_{\theta\theta} = \dfrac{u_r}{r}$)

Outlook for this week

Find your way to the **online book** (for weeks 1–4):

- `https://interactivetextbooks.citg.tudelft.nl/computational-modelling`
- `Course schedules - CIEM1110`: tailored reading guide
- `Codes - Pyjive`: dowload link for python code
- Chapter `Introduction to finite elements`: study before Thursday

On **Wednesday** will be the first of a series of interactive workshops

- Introduction to `pyjive`
- See the structure of a more general FE code than the single purpose scripts from MUDE
- We will use this code for workshops in weeks 1–4 and for the viscoelasticity assignment

Thursday will be another lecture including review of MUDE material

- Prepare by studying book material
- There will be space for your questions
- We will show how to derive the FE formulation for the PDE $\nabla \cdot \boldsymbol{\sigma} + \mathbf{b} = 0$