11-7-2017

Image analysis, synthesis and image-based modeling of ceramic-matrix composites

Gerard L. Vignoles
University of Bordeaux, France, vinhola@lcts.u-bordeaux.fr

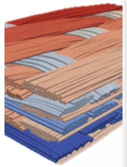
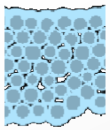
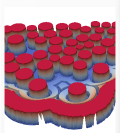
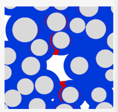






IMAGE ANALYSIS, SYNTHESIS AND IMAGE-BASED MODELING OF CERAMIC-MATRIX COMPOSITES

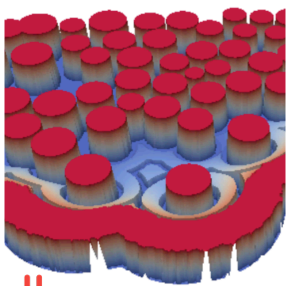
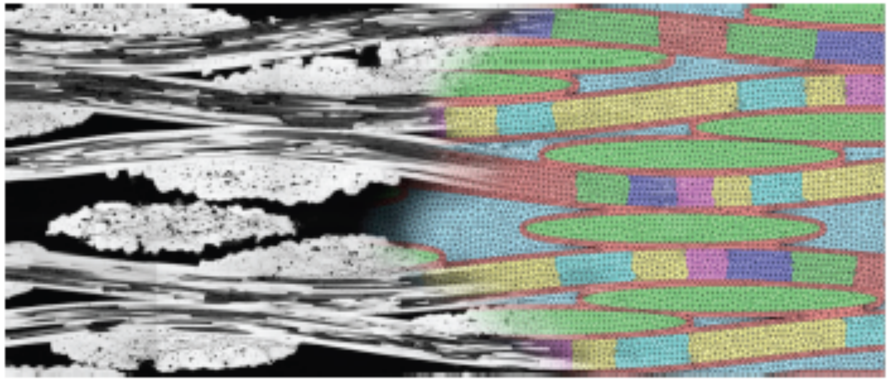
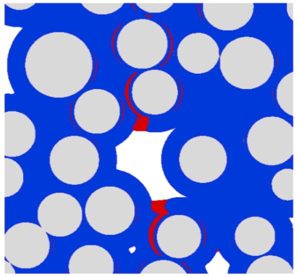
… some research by the

Laboratory of Thermostructural Composites

UMR 5801

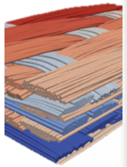
CNRS-Safran-CEA-Université de Bordeaux

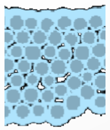
Gerard L. Vignoles

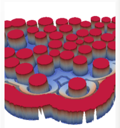




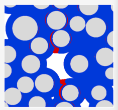
The ECI CMC Conference, Santa Fe, NM, Nov. 2017

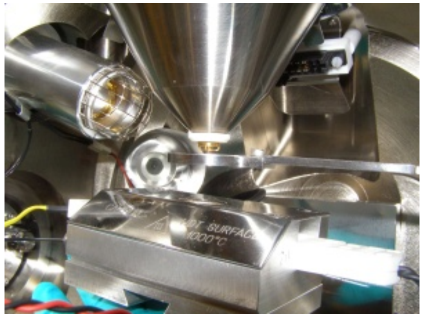
Laboratory for ThermoStructural Composites

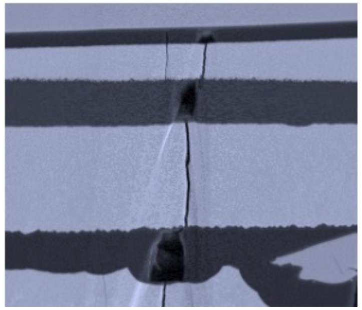


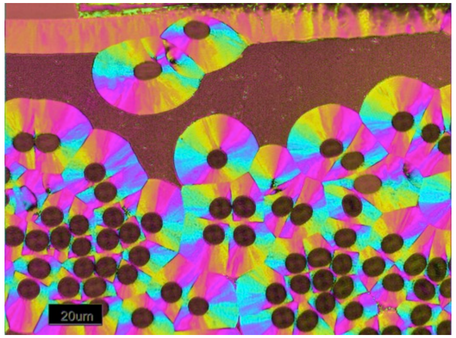


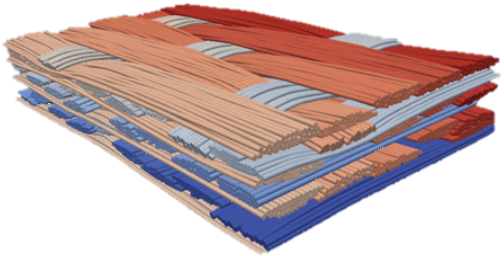


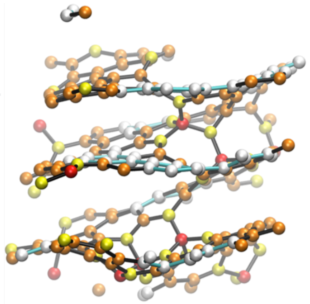


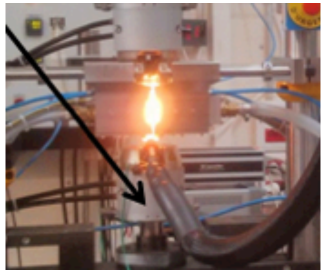










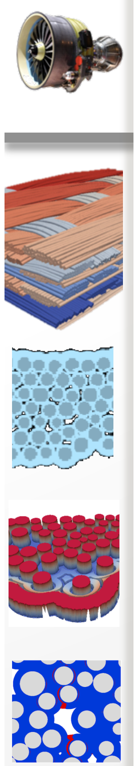


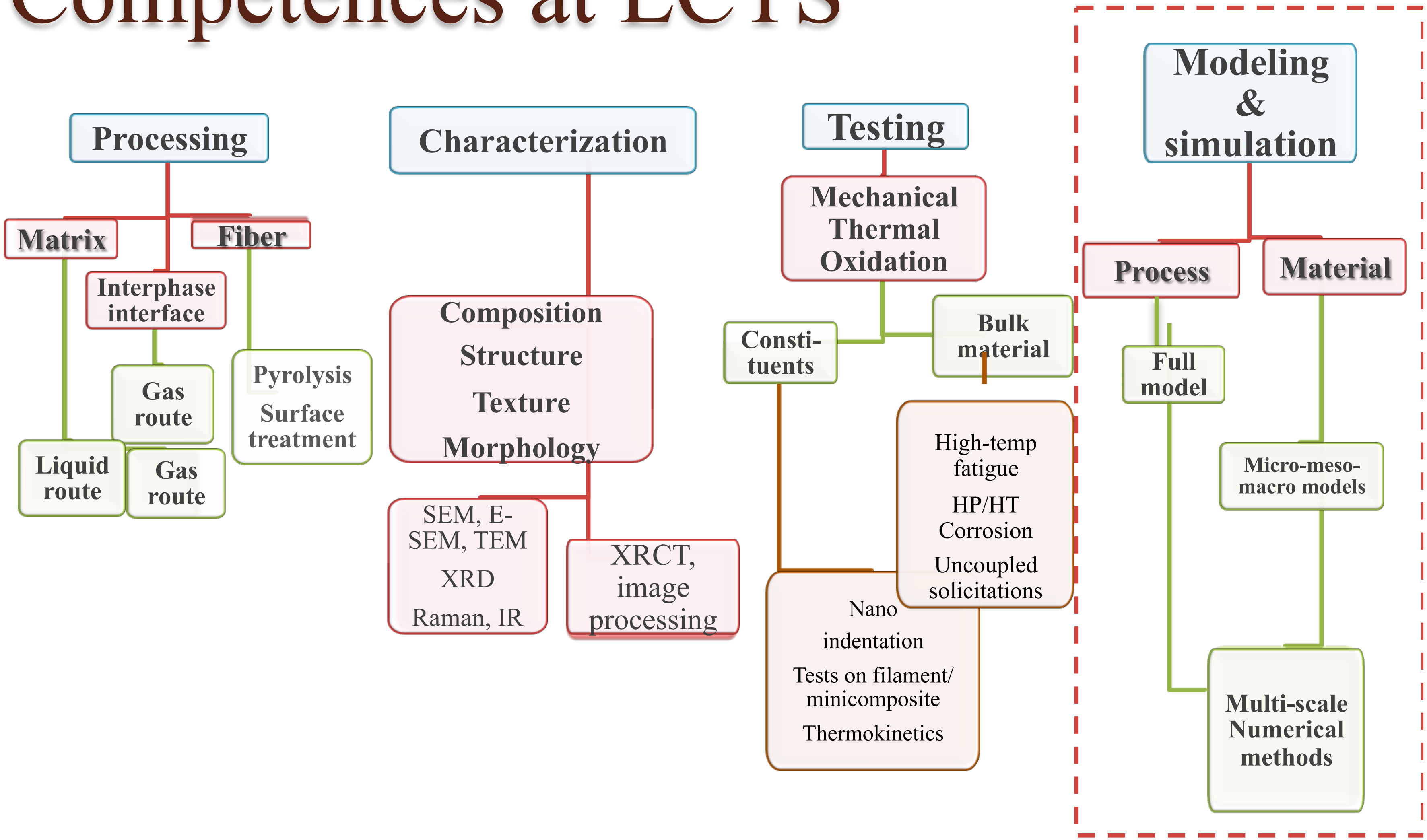
Founder : Pr. Roger Naslain (1988)

Joint research unit UMR5801 created in 1988, 4 partners:

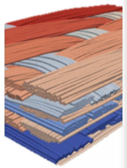
- **Centre National de la Recherche Scientifique (CNRS)**
- **Université de Bordeaux (UBx) - Science & Technology**
- **Safran**
- **Atomic & Alternative Energies Agency (CEA, 1999)**

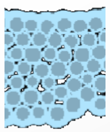
Competences at LCTS

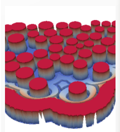


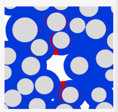


Outline







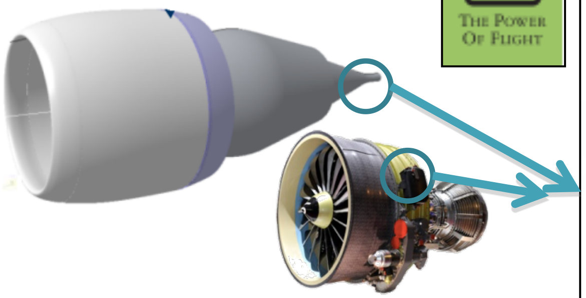


- Context
- Image analysis & synthesis
- Modelling Gas-phase Infiltration of Ceramic Matrices
- Modelling evolution under high-T oxidation
- Modelling mechanical behavior
- Conclusion & perspectives

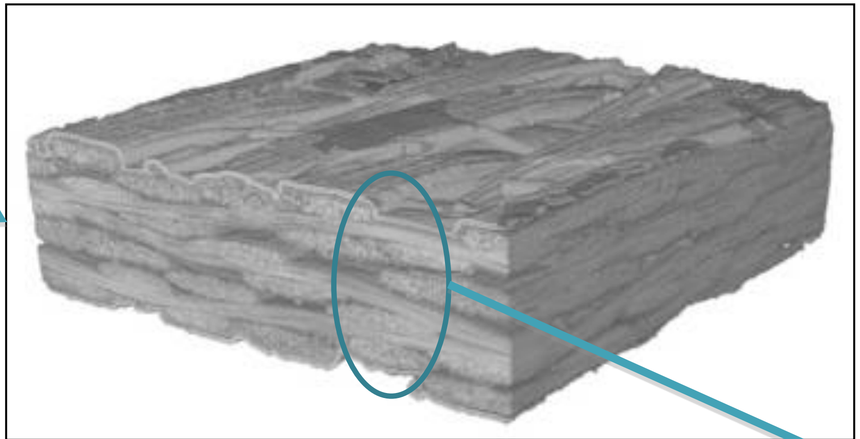
Part 1

CONTEXT

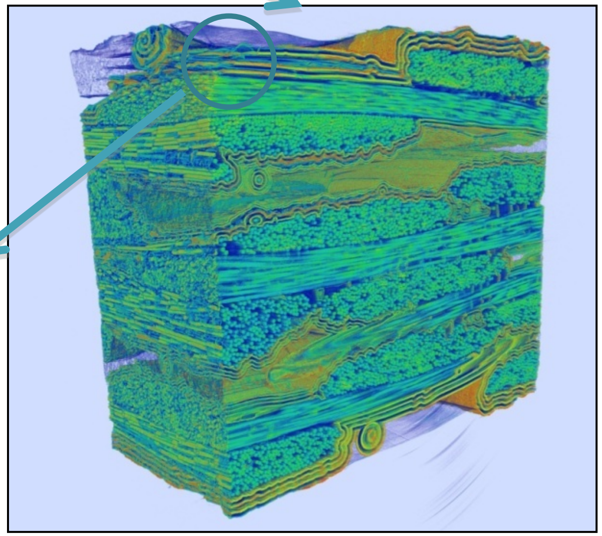
CMCs in new-generation aircraft engines



Aircraft engine parts



Woven 3D architecture



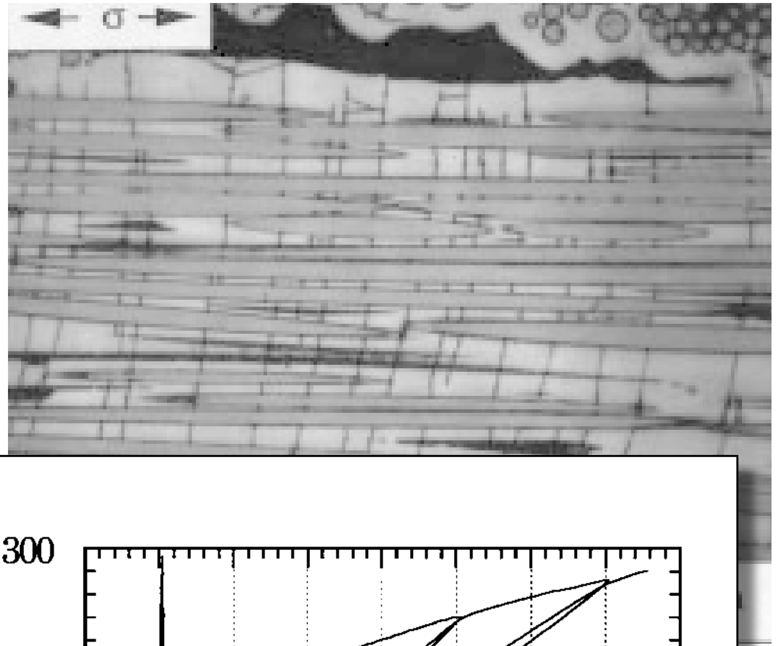
Silicon & boron carbide based multilayer matrix

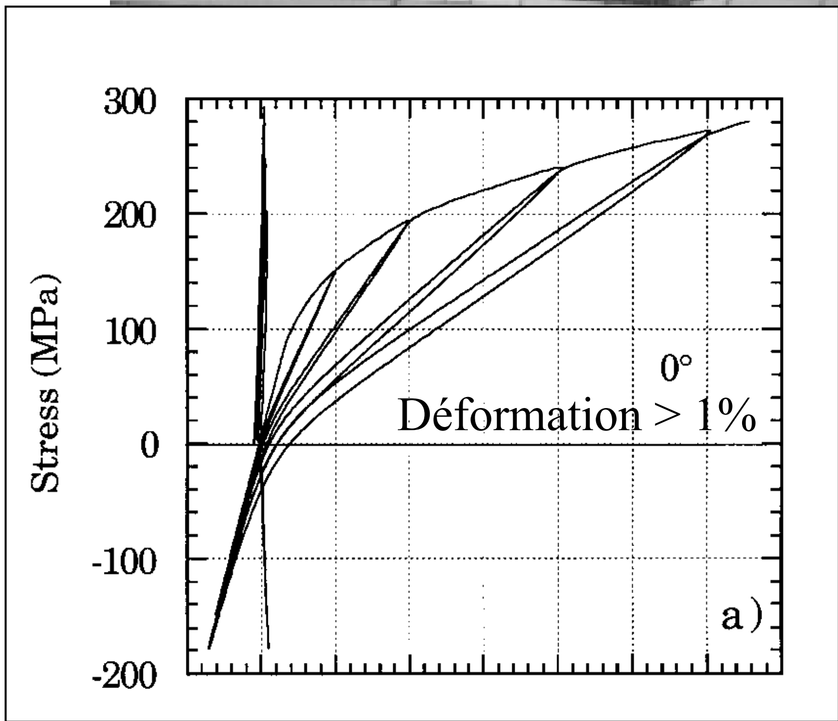
Carbon/ SiC fibers

Ceramics → lighter, more refractory → energy savings, less pollution

Ceramic Matrix Composites (CMCs)

- **Ceramic fibers** : high modulus & strength, even at high T
- **Ceramic Matrices** : Stiff & strong, Compatible with fibres
- All components are brittle! But matrix multicracking occurs
- Interphases : crack deviators
- Cracks = paths for corrosion
- Protective layers inserted in matrix





G. Camus, 1996

Motivations, objectives

- High standard materials, costly fabrication
- Need to guarantee performances
- Need to optimize production without increasing, or lowering costs

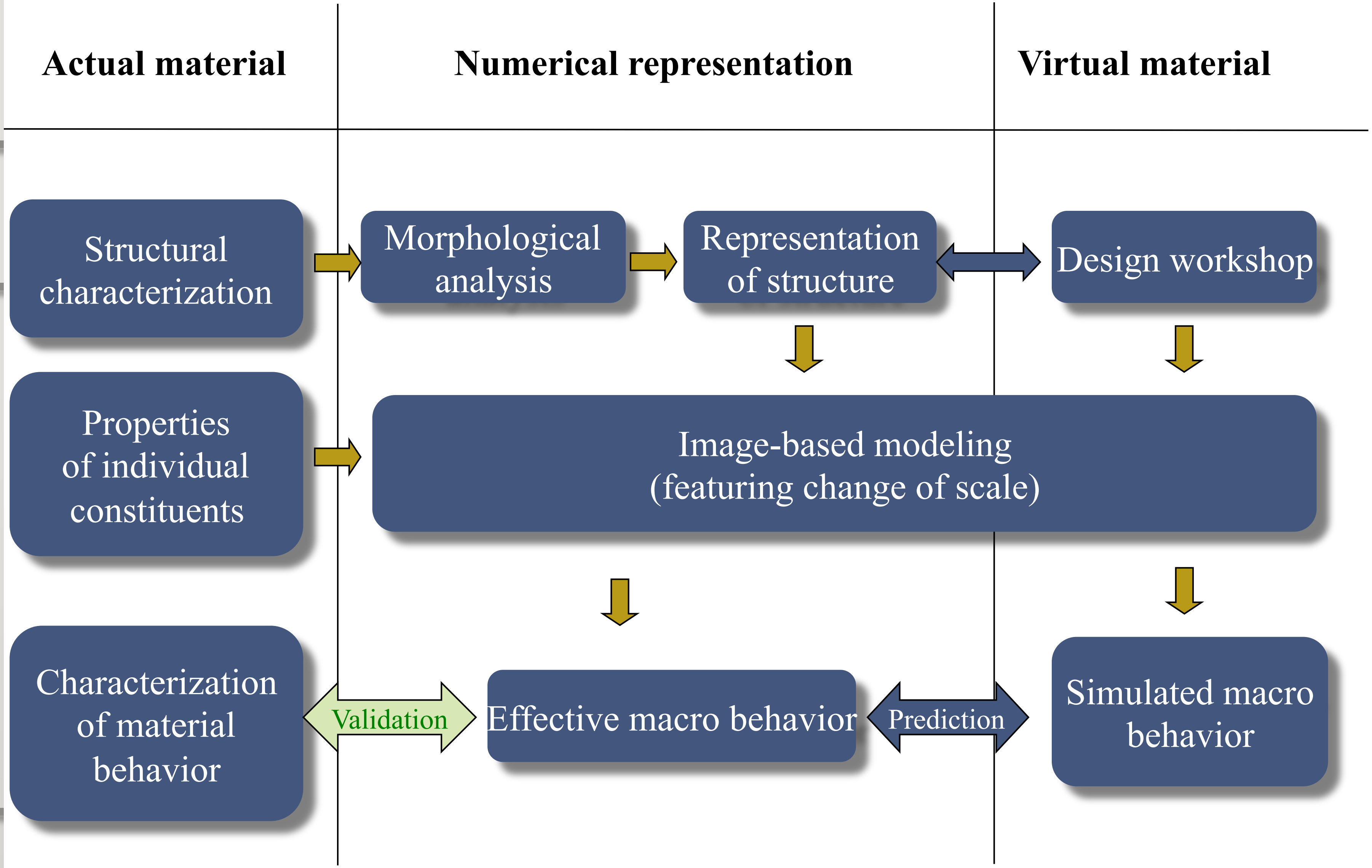
➡ Pertinence of numerical simulation & of ***validated*** modeling

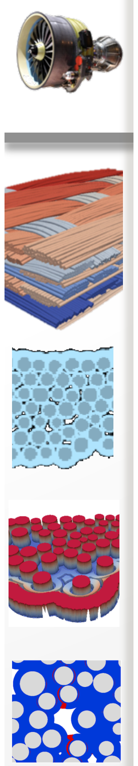
➡ Handling NUMERICAL / VIRTUAL materials & processes

Before going virtual … be actual !

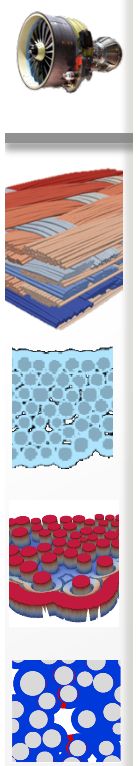
- Try & describe the material *as it is*
  - Morphological analysis
  - «Non-destructive » characterization
- Extract descriptors to feed an « *in silico* » material synthesis
- *Validate experimentally* the behavior simulated from constituents and their arrangement
- Varying descriptors enables *optimizing* virtual materials

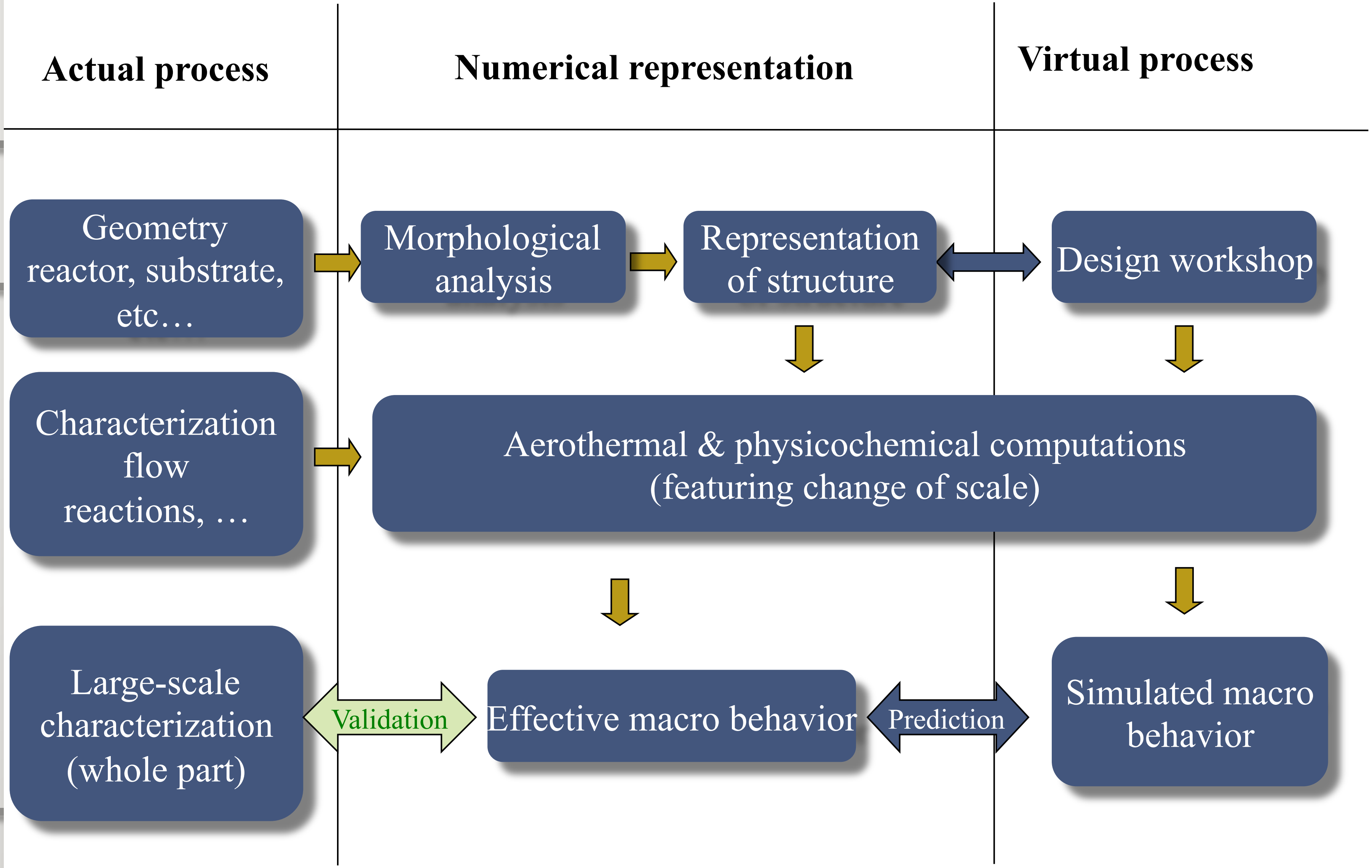
Virtual material strategy



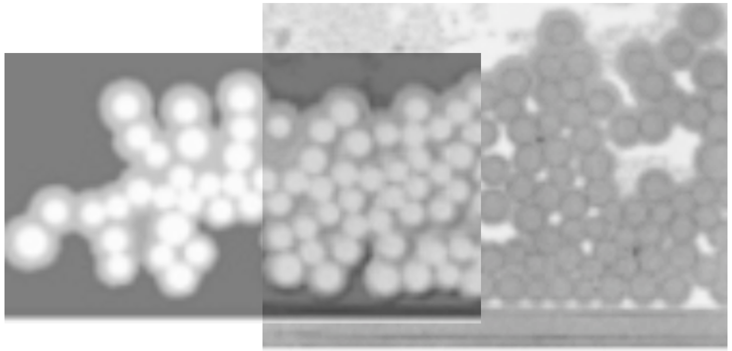


Virtual process strategy



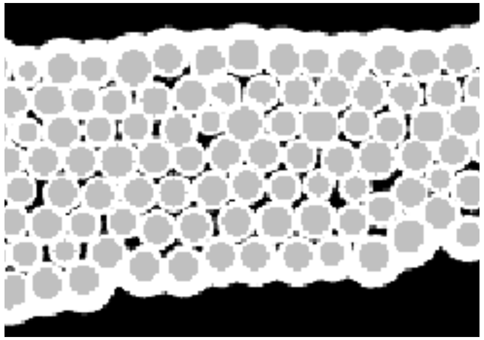


Modeling activities

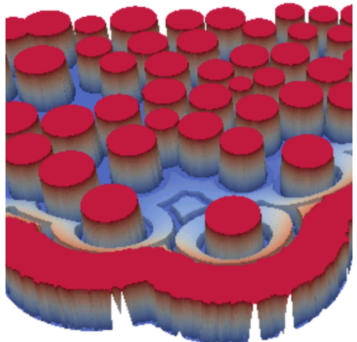


CMC imaging & analysis

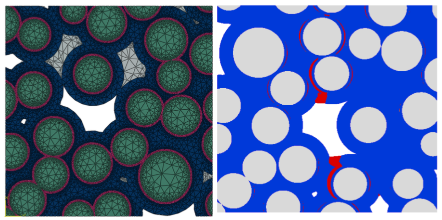
Infiltration modeling



Self-healing modeling



Mechanical modeling



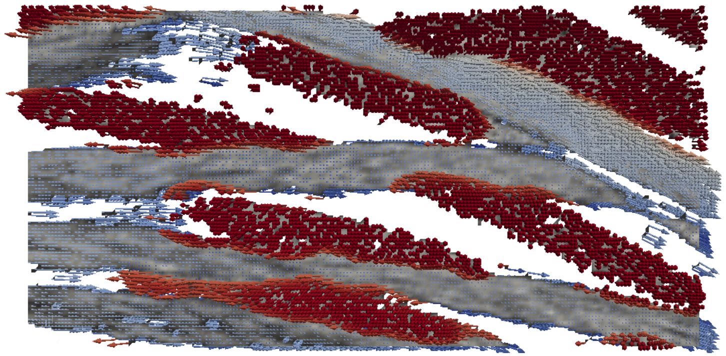
Part 2

IMAGE ANALYSIS & SYNTHESIS

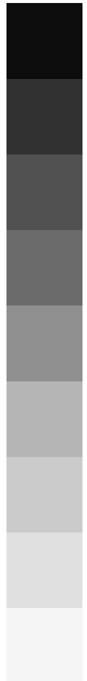
Detecting orientations in images

$$\underline{\underline{T}} = \begin{pmatrix} \left(\frac{\partial I}{\partial x}\right)^2 & \frac{\partial I}{\partial x}\frac{\partial I}{\partial y} & \frac{\partial I}{\partial x}\frac{\partial I}{\partial z} \\ \frac{\partial I}{\partial x}\frac{\partial I}{\partial y} & \left(\frac{\partial I}{\partial y}\right)^2 & \frac{\partial I}{\partial y}\frac{\partial I}{\partial z} \\ \frac{\partial I}{\partial x}\frac{\partial I}{\partial z} & \frac{\partial I}{\partial y}\frac{\partial I}{\partial z} & \left(\frac{\partial I}{\partial z}\right)^2 \end{pmatrix} = P^{-1}.diag(T).P$$

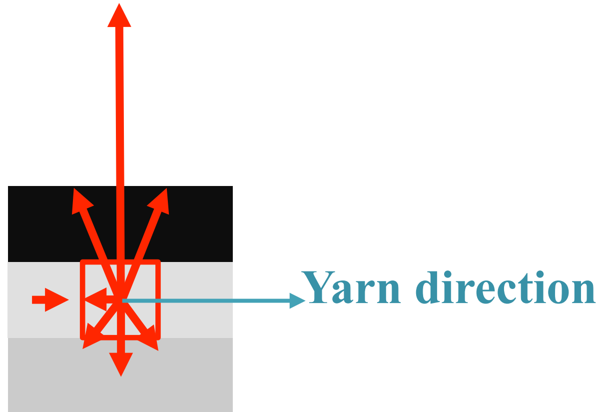
Image structure tensor



μCT



Grayscale level gradient



2D example

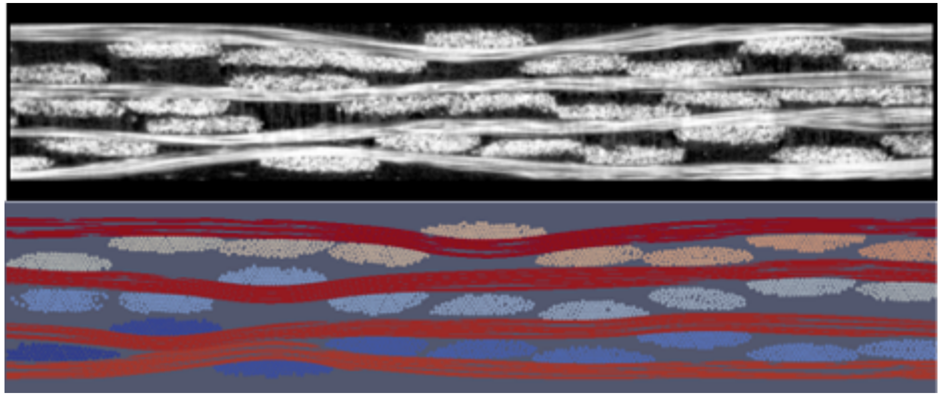
☺ Fast & automatic

☺ Image-based : realistic

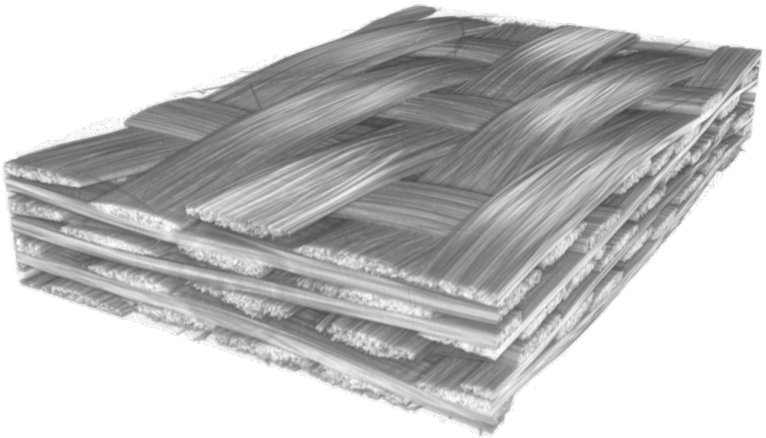
— Notion of yarn

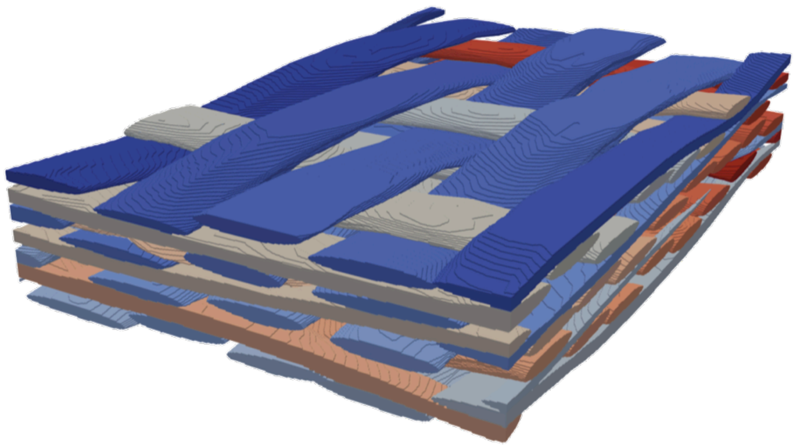
— Highly dependent on CT scan quality

Yarn retrieval software : GenDir



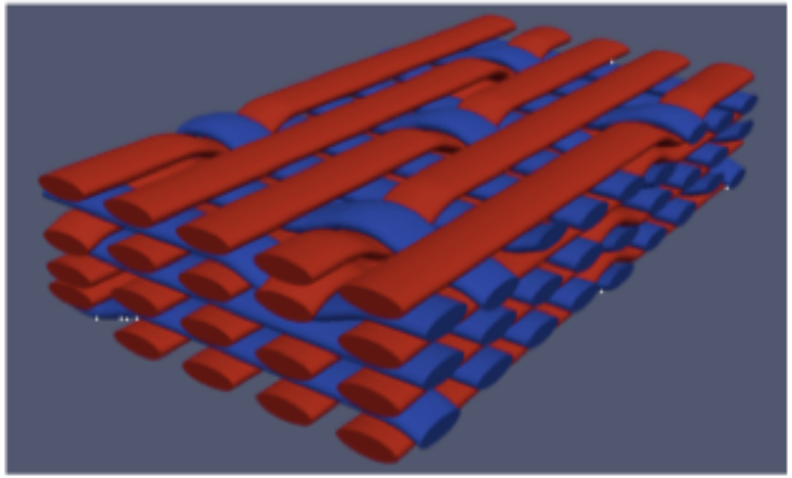
New method under development : image-guided relaxation
⇒ Minimal manual operation
⇒ More robust
⇒ Avoids interpenetrations



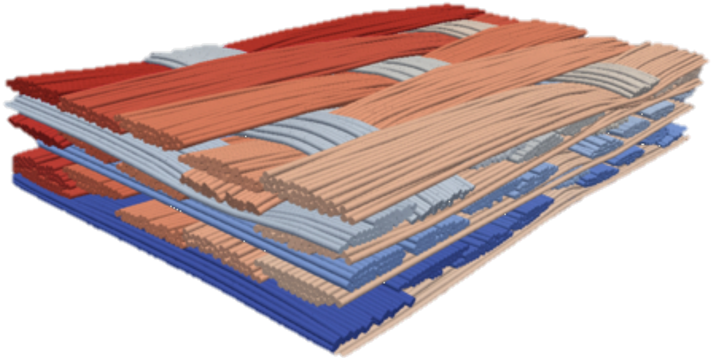


Macro-wire virtual weaving: GenFil

3D weaving:
Geometric model,
with appropriate topology



Intermediate model made of macro-wires subject to mechanical equilibrium



G. Couégnat, H. Ayadi, C. Saurat, "Towards realistic geometric modeling of woven fabrics", Proc. 19th International Conference on Composite Materials (ICCM19), Montreal, 2013.

Synthesis of fibers in a yarn

Uses an « object dynamics » algorithm (Verlet) for a 2D slice
+ Continuation in 3D

C. Chapoullié, PhD diss.
U. Bordeaux (2015)

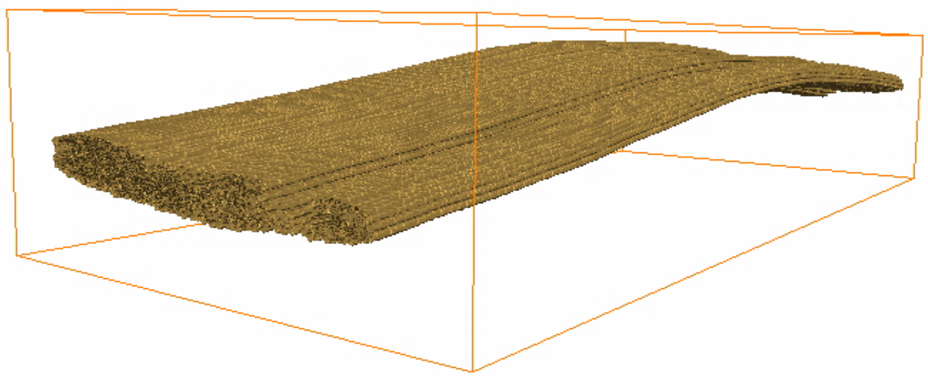


Image processing : summary & outlook

Numerical tools & strategy

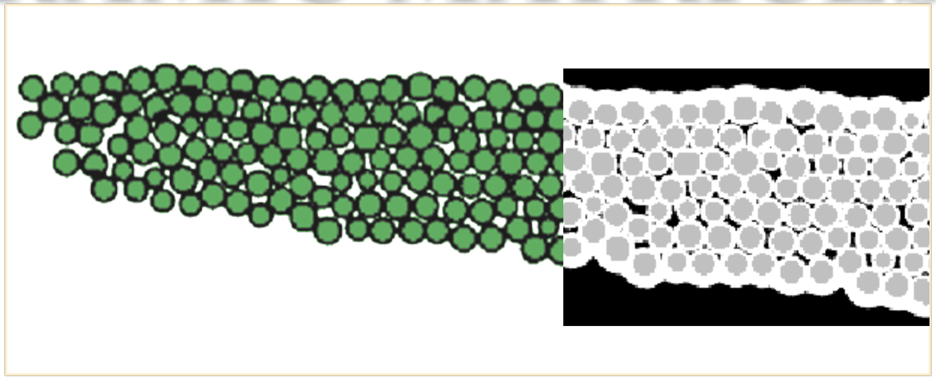
- Orientation detection is a key tool
- 2-scale work
- Efficient software tools, now transferred to industry
- The next question is: how to transfer to numerical simulations ?

Outlook

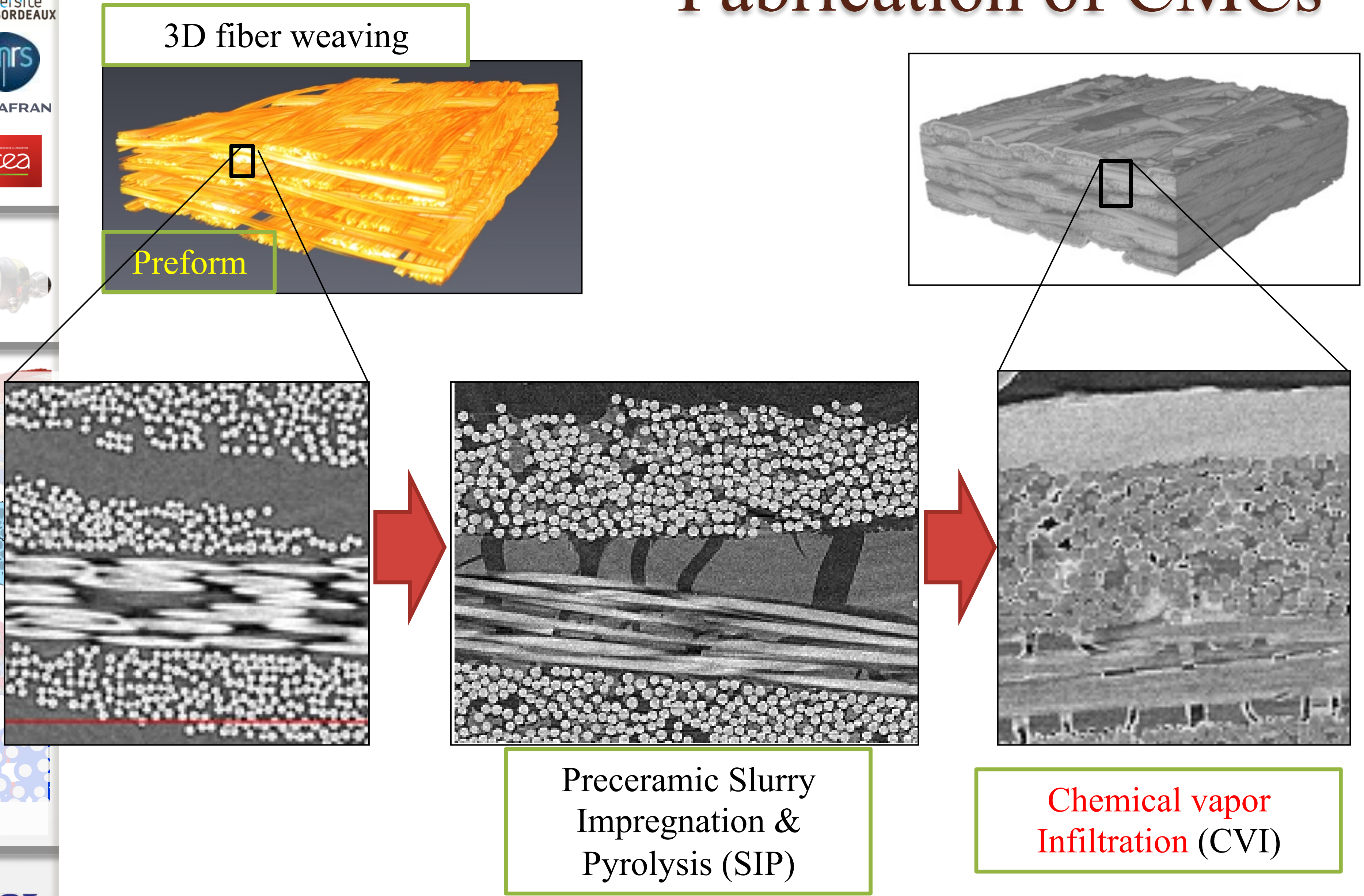
•Improving the robustness & CPU/memory demand of the methods

Part 3

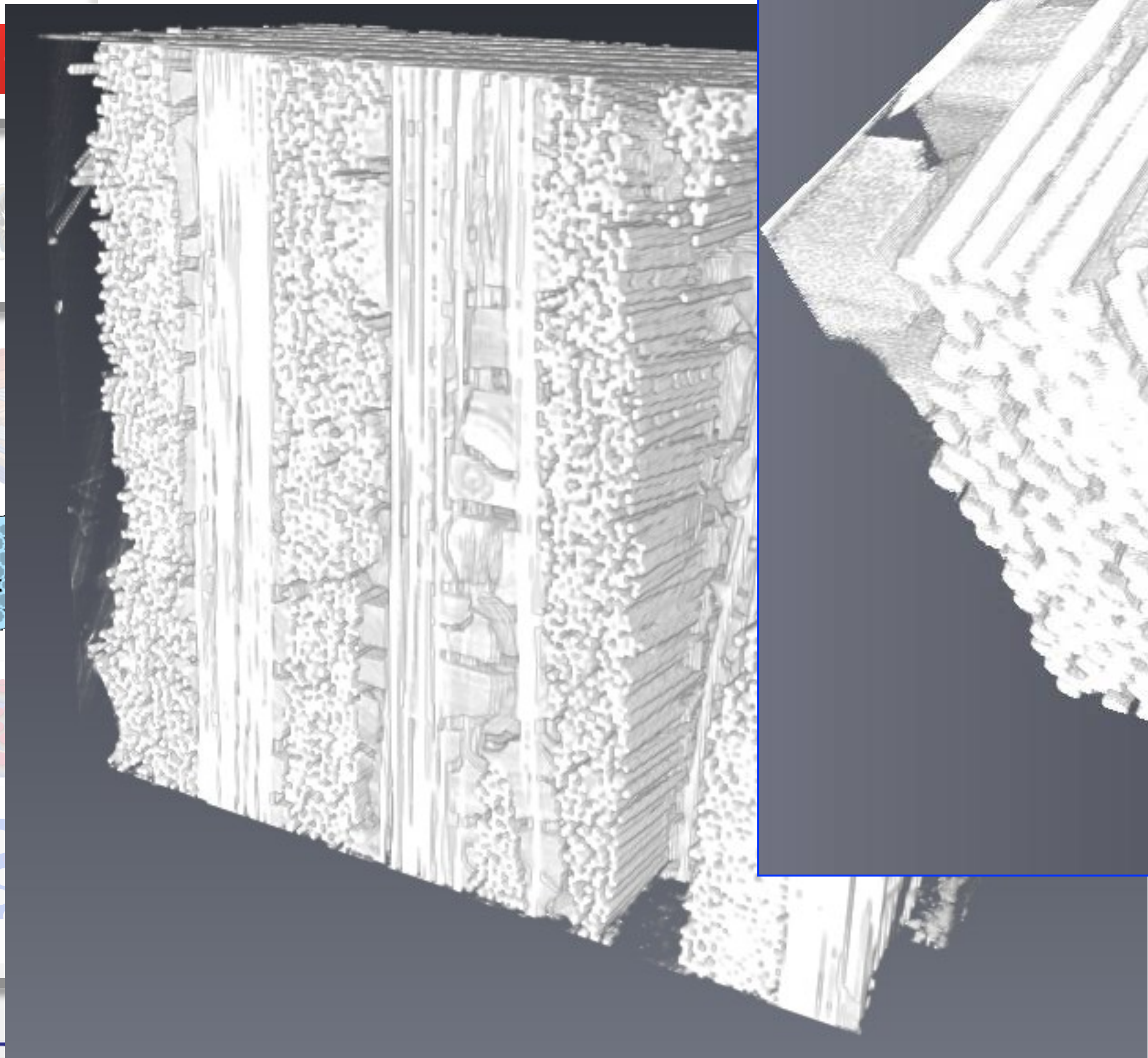
MODELLING OF GAS-PHASE INFILTRATION OF CERAMIC MATRICES

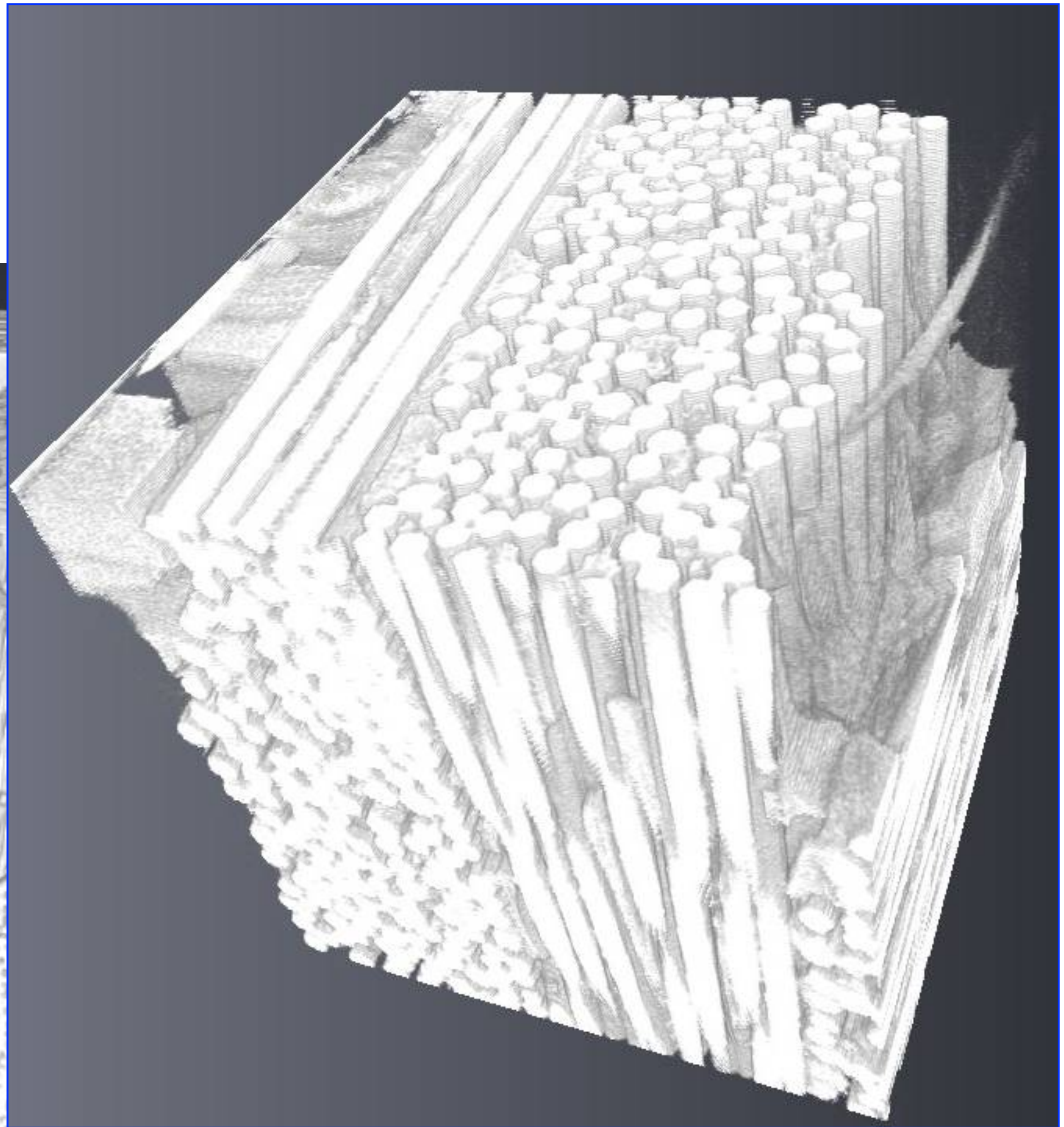


Fabrication of CMCs



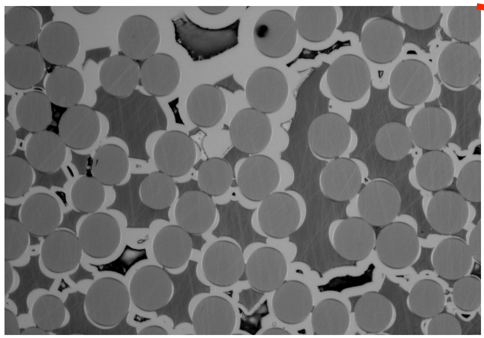
Fibers + SIP matrix

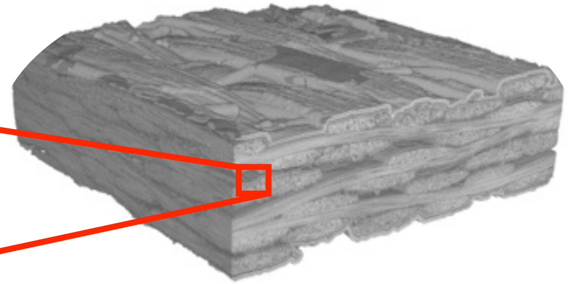




How "infiltrable" is this ??

Modeling strategy





Composite scale

Fiber scale

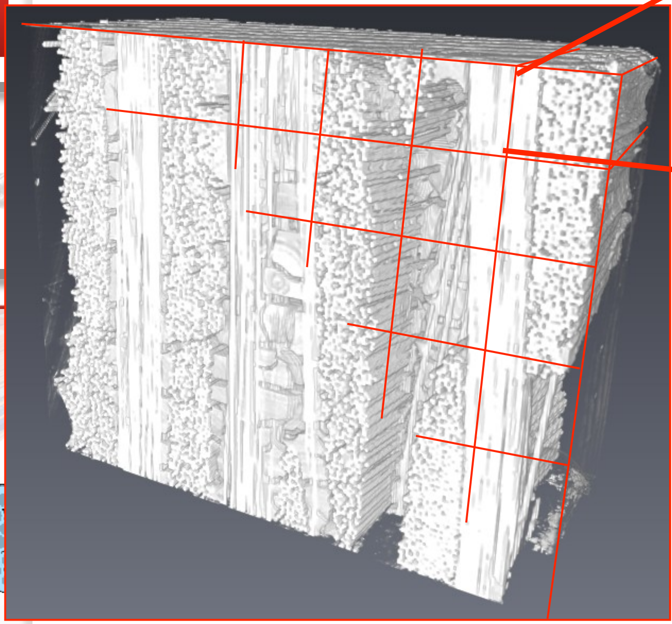
Change of scale

- Acquisition & processing of **tomographic images**
- Development of two software “porous media” codes : **fiber scale & composite scale**
- **Connection** of the two codes through effective laws

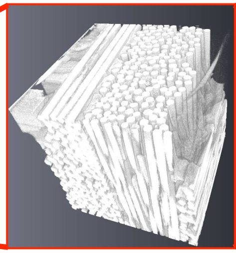
G. L. VIGNOLES, W. ROS, C. GERMAIN,
Ceram. Eng. Sci. Procs., **34**(10), 267-271 (2014).

2-scale modeling strategy

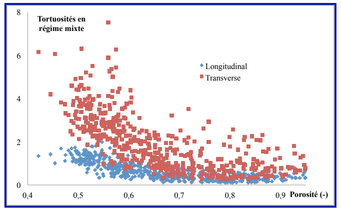
High-resolution tomograph



Splitting into sub-volumes

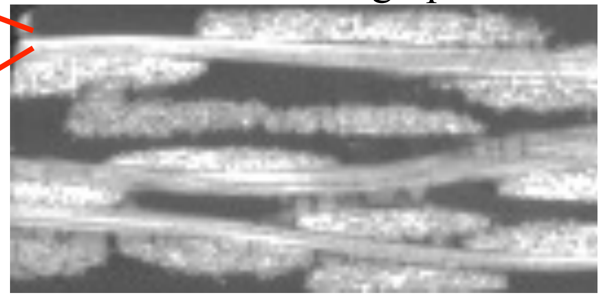


Computation of
properties
in each subvolume



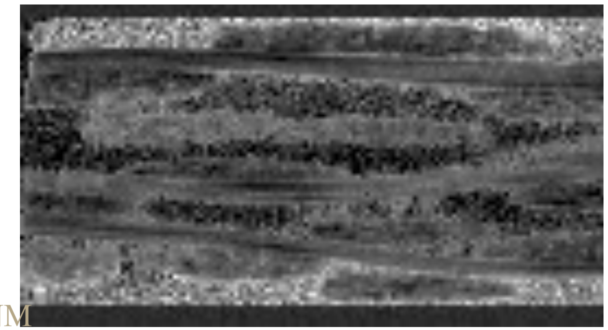
Laws : Props = f(poro)
+ statistics of dispersion

Low-resolution tomographs



Identification of porosity
& fiber orientation
Injection of laws

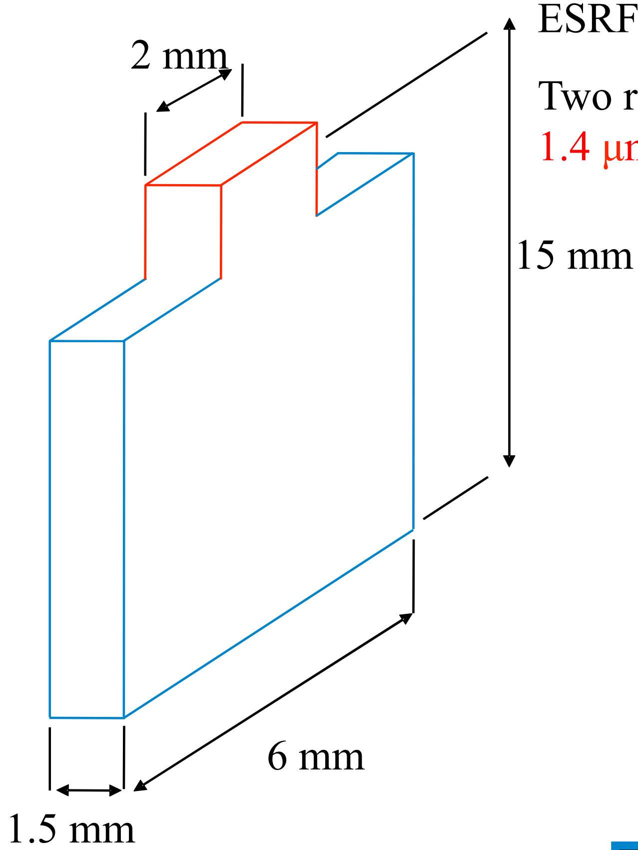
Infiltration simulation over whole
width of the composite part

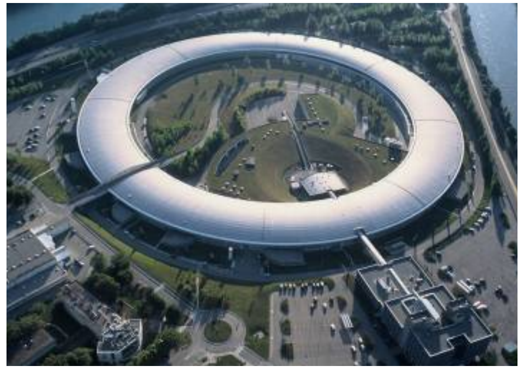


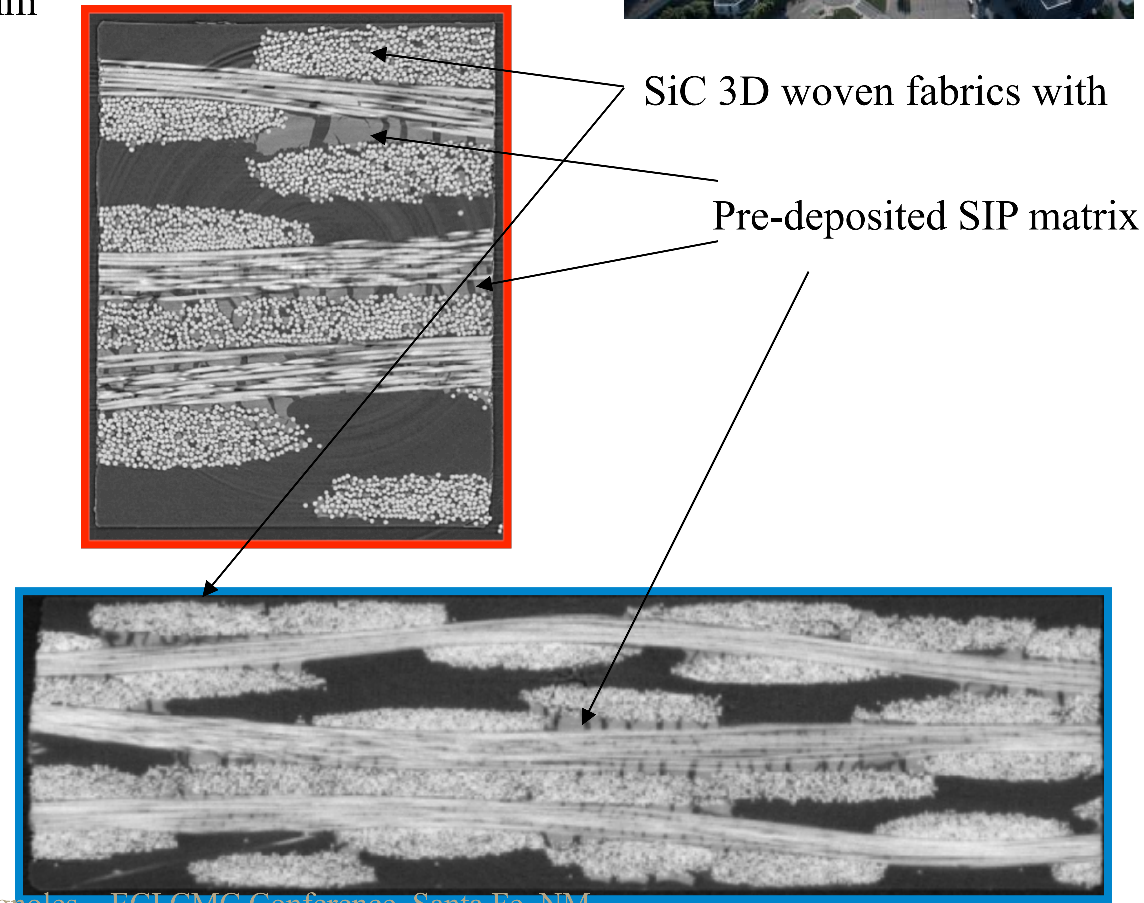
Investigated preforms

Images acquired by X-ray CMT :
ESRF ID19 line

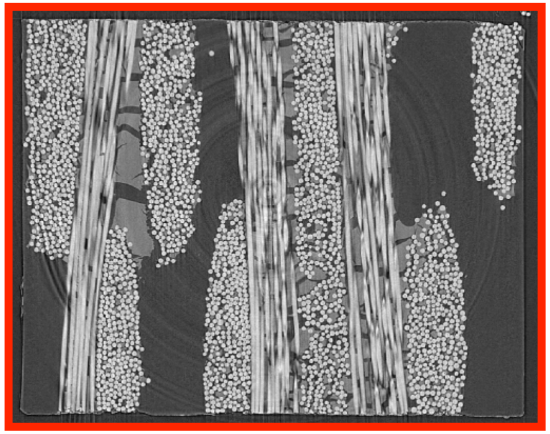
Two resolutions for acquisition :
1.4 µm/pixel and 5 µm/pixel





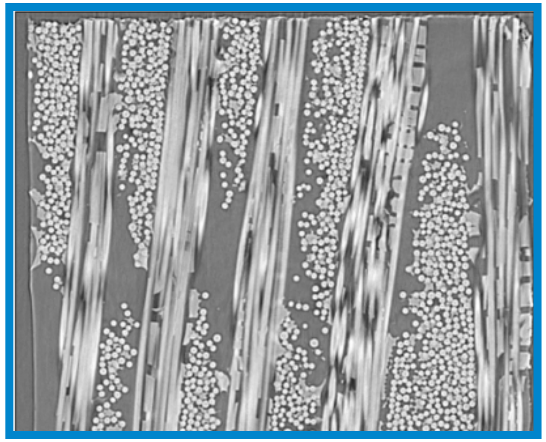


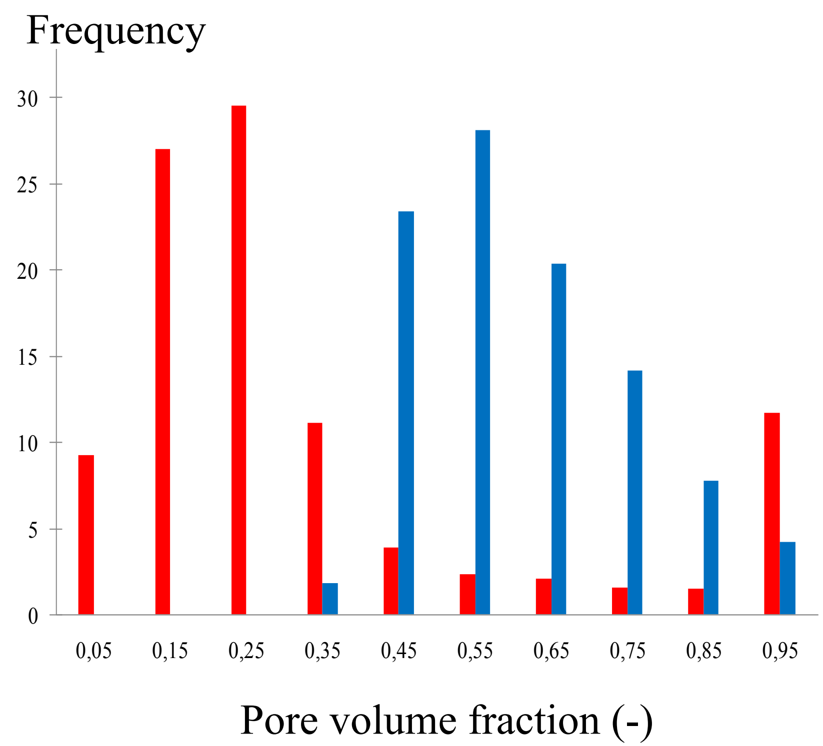
Two distinct fibrous arrangements

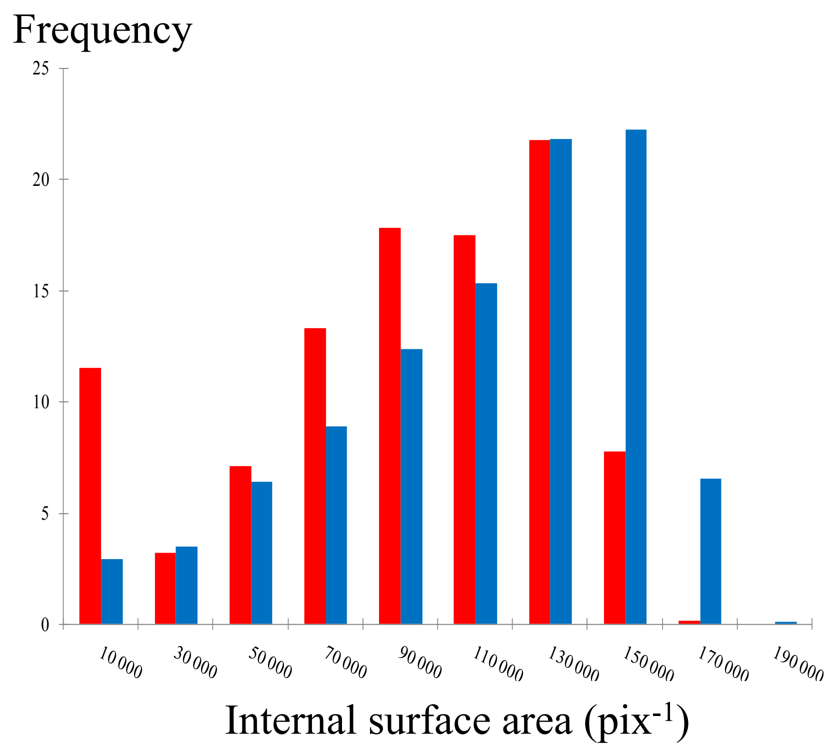


Preform **M1**

Preform **M2**

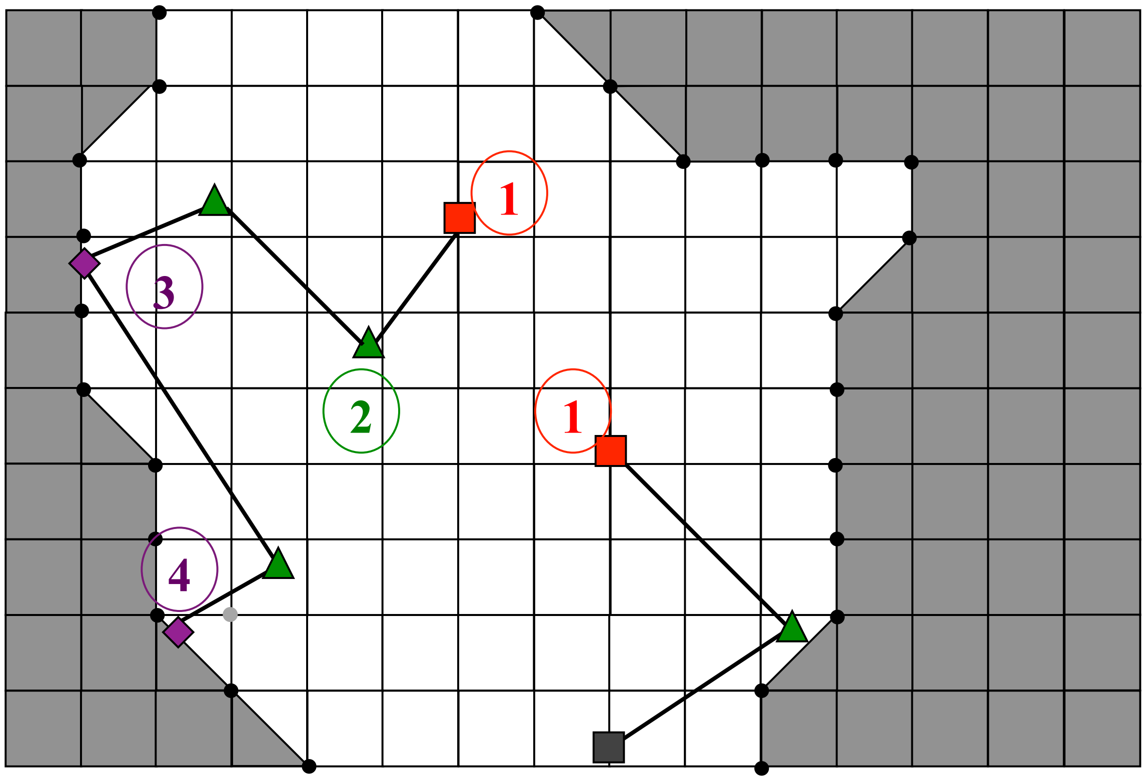






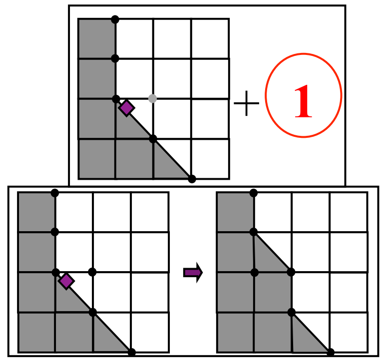
Fiber-scale infiltration modeling : DMC

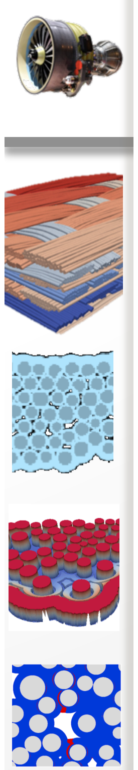
« Kinetic » Random walk w/ reaction and surface growth



Legend: ■ Random position and direction — ▲ Binary collision — ◆ Wall collision — ✕ Voxel borders — ■ End of time process

1. **Start of time process**
   Random position
   Random direction
   Isotropic distribution
2. **Binary collision**
   Time until next collision
   Random direction
   Isotropic distribution
3. **Wall collision without reaction**
   Random direction
   Knudsen's cosine law
4. **Wall collision with reaction**

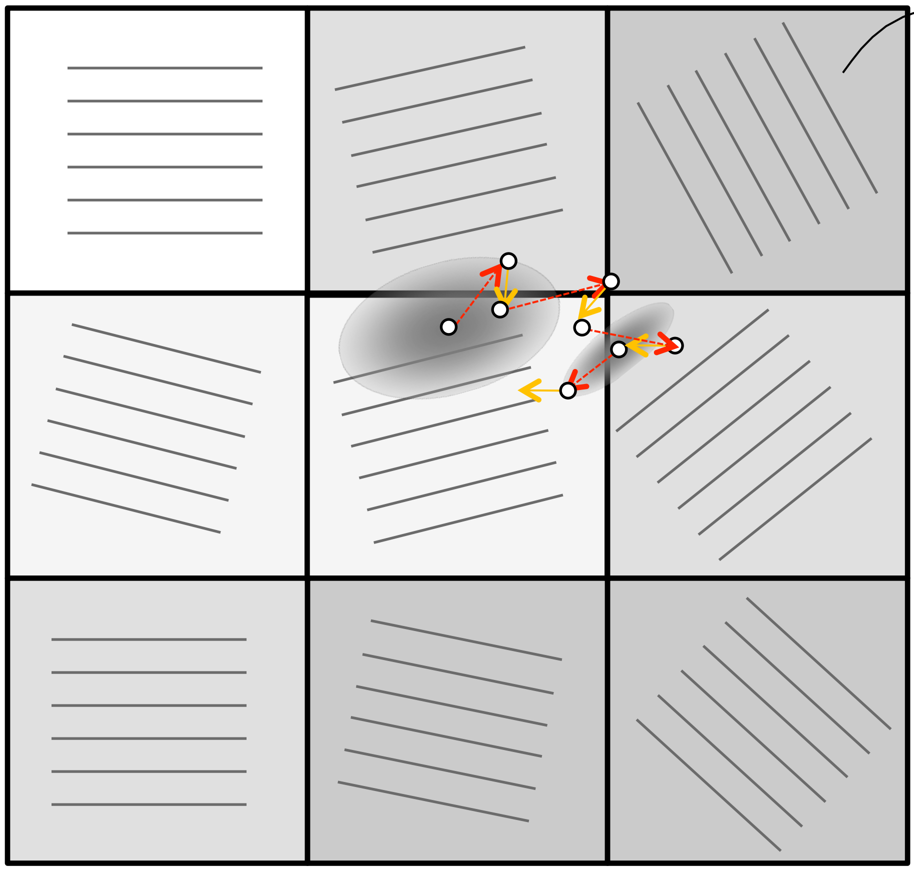




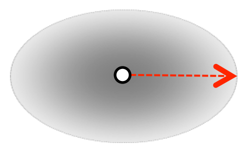
G. L. VIGNOLES, W. ROS, C. MULAT, O. COINDREAU, C. GERMAIN, *Comput. Mater. Sci.* **50**, 1157-1168 (2011)

Large-scale infiltration modeling : LIRWa

- Itô-Taylor random walks



Diffusion tensor D computed in each voxel from greyscale value (density) and local fiber orientation



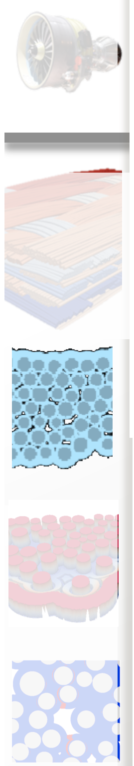
Diffusive step : random direction w/ anisotropic Gaussian distribution following D

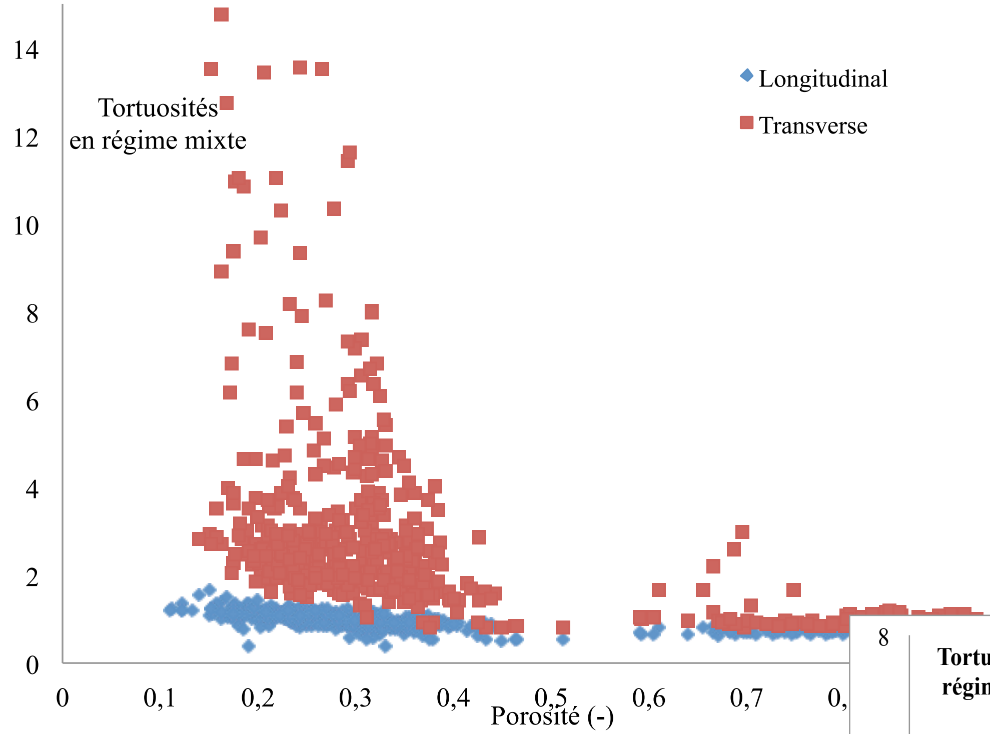
Advective step following *div.D* (heterogeneity)

« Russian roulette » for deposition reaction

G. L. VIGNOLES, W. ROS, I. SZELENGOWICZ, C. GERMAIN, *Comput.l Mater. Sci.* **50**, 1871-1878. (2011)

Gas diffusion – intermediate regime



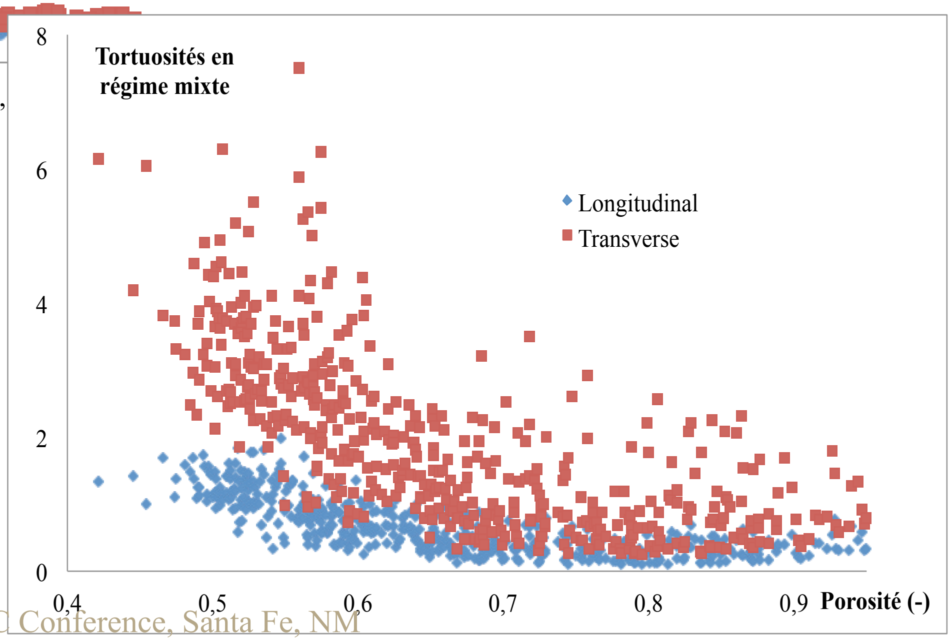


$$\eta = \frac{\eta^{bin} + Kn.\eta^{Kn}}{1 + Kn}$$

Intermediate regime tortuosities (Kn = 0.3)

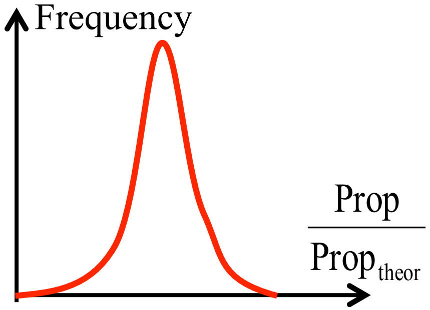
Preform M1

Preform M2

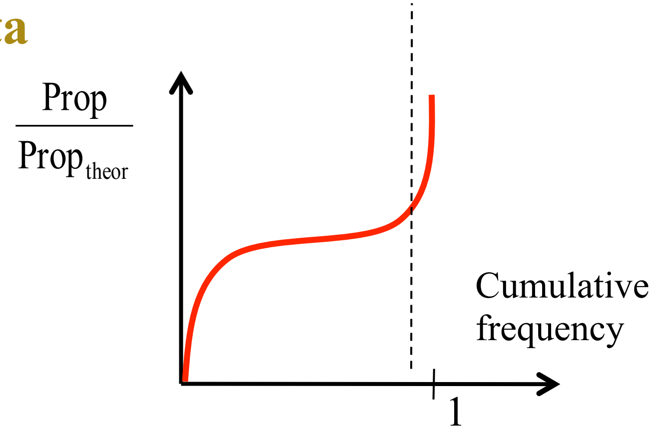


Incorporating dispersion

Injection of the observed statistical data



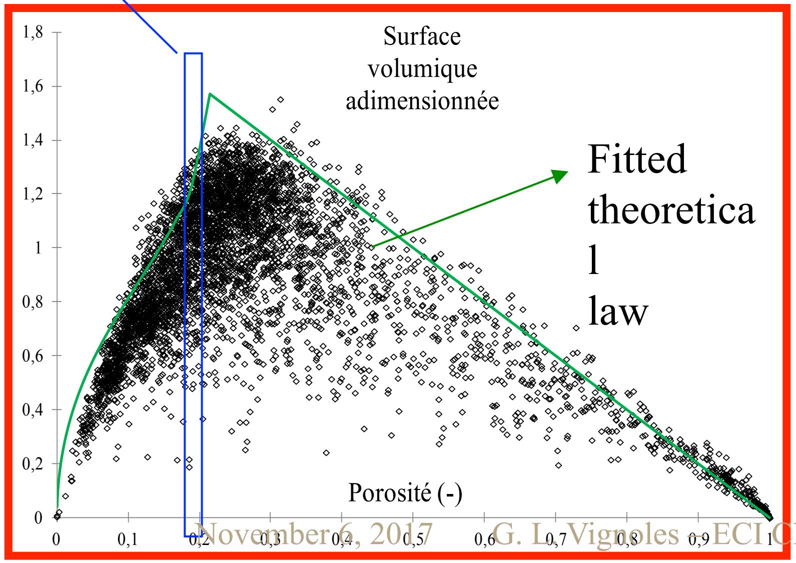
Computation of the ratio between actual value and fitted law value

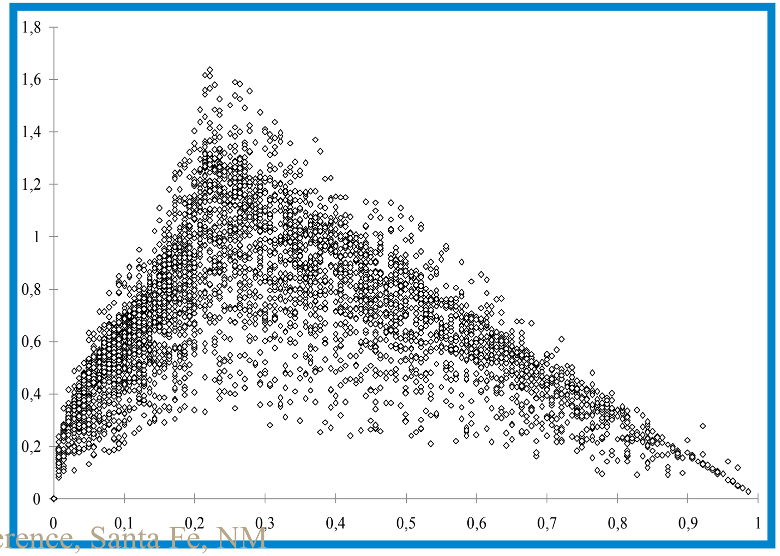


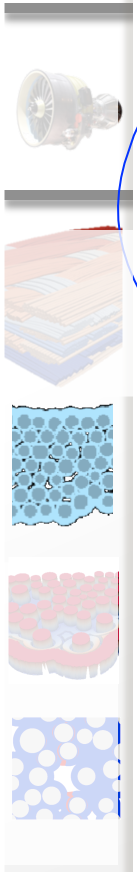
Computation of the cumulative frequency and of its reciprocal fctn.

At large scale : theoretical value is biased by a random drawing with injected cumulative frequency

Validation : distributions from actual micro scale and computed macro scale are equivalent







Simulation of infiltration

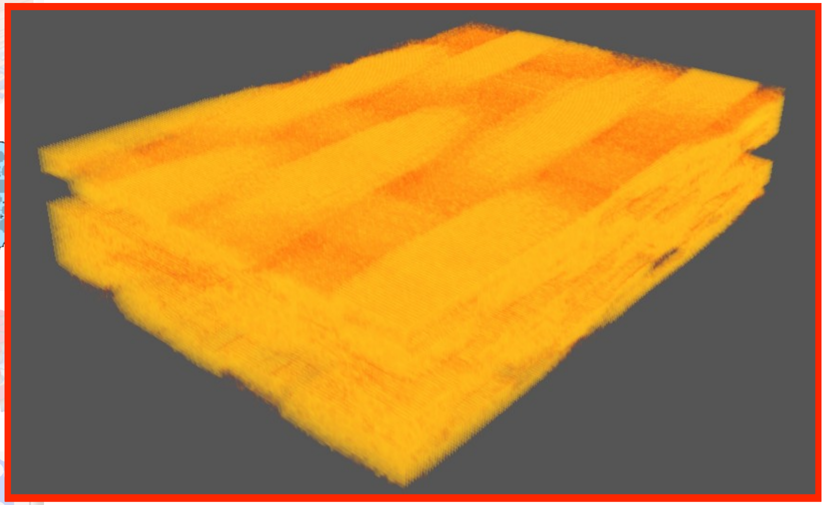
Integration of the effective laws + dispersion in macroscale solver

Downgrading the macroscale tomographs resolution → **computational time savings**

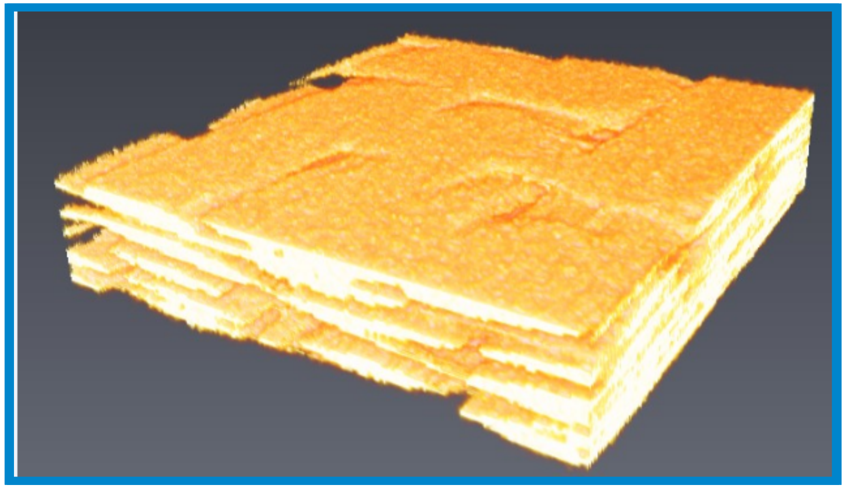
Infiltration simulations for different values of the **heterogeneous reaction constante**

Comparison of **macroscopic properties** of each preform

Preform M1

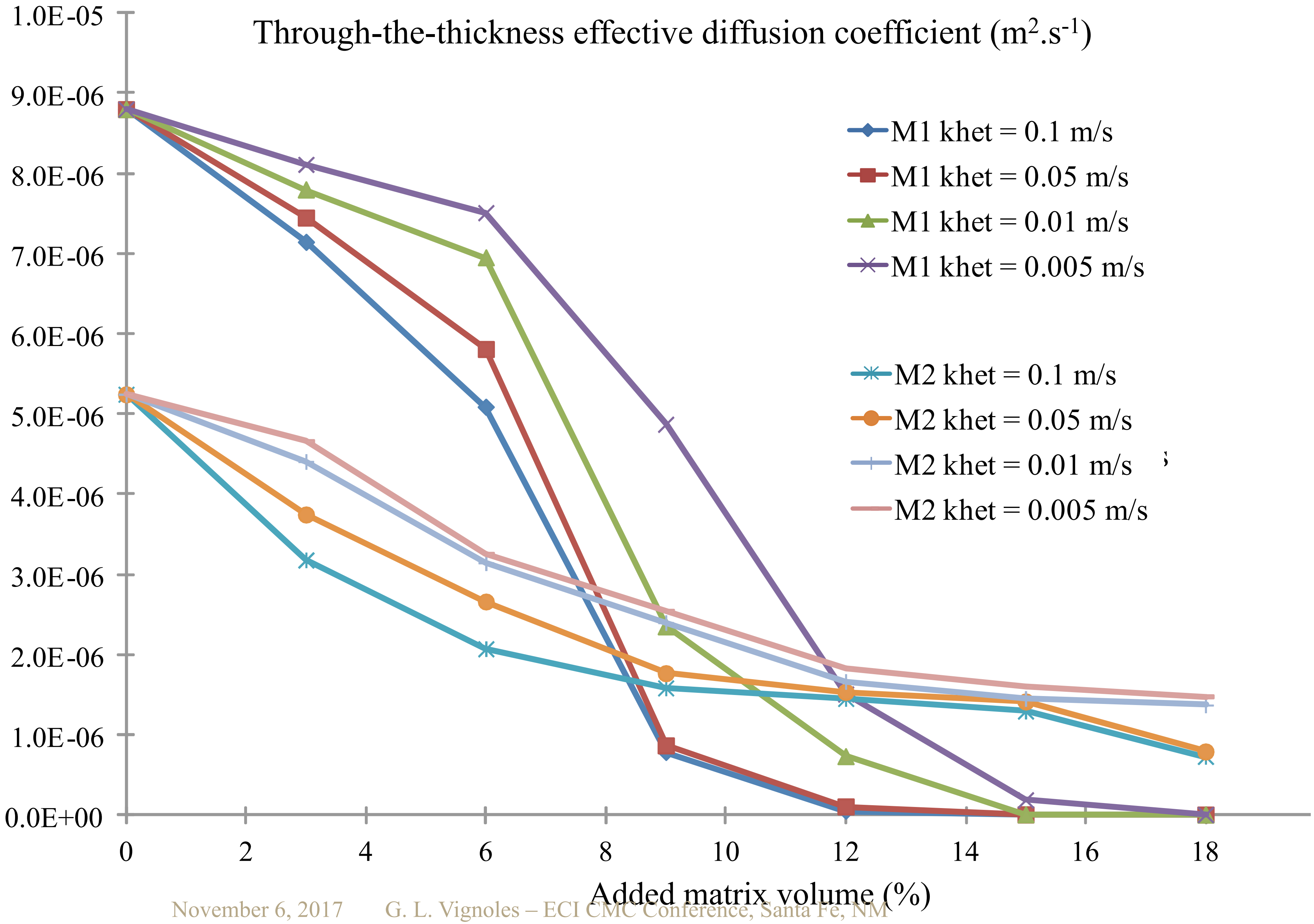


Preform M2

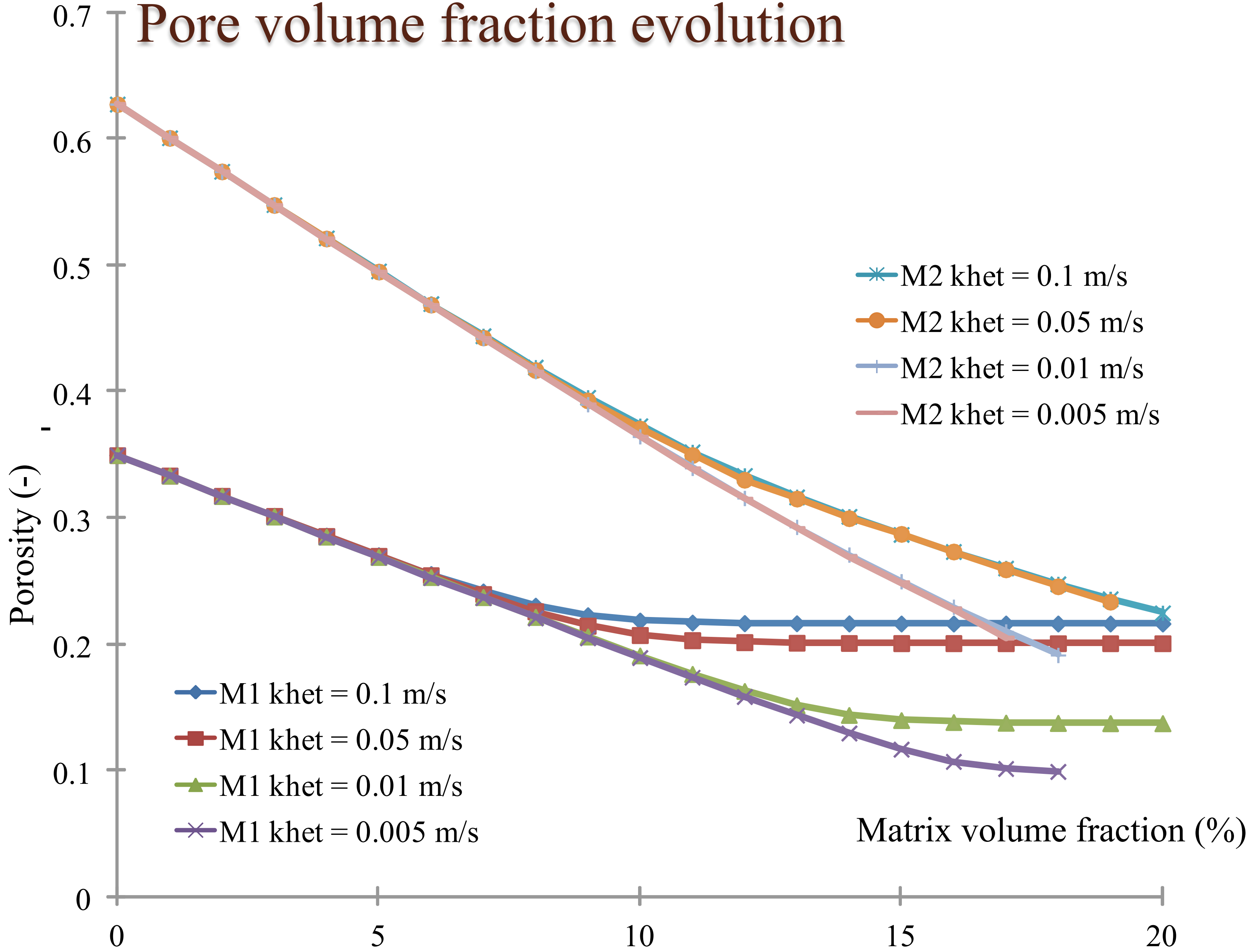


G. L. VIGNOLES, W. ROS, C. GERMAIN, in *Ceram. Eng. Sci. Procs.*, **34**(10), 267-271 (2014).

Diffusivity evolution

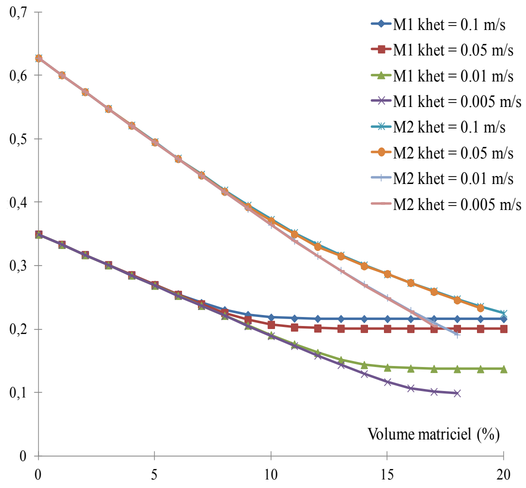


Pore volume fraction evolution

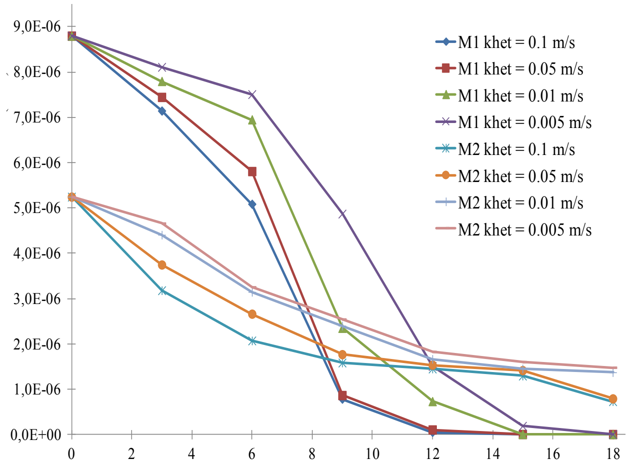


Discussion

Pore volume fraction evolution



Effective diffusivity evolution



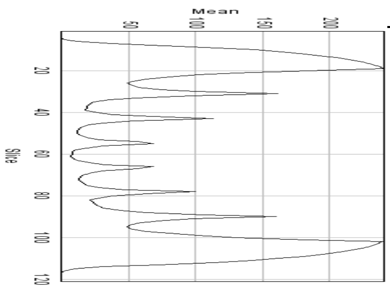
M2 has a better « infiltrability » than M1

Whatever the processing conditions, **preform M1 gets plugged faster** than preform M2

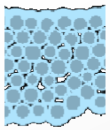
The microscale conclusions are **verified** at the composite scale

Identification of the parameters controlling infiltrability → An efficient engineering tool

Modeling Chemical Vapor Infiltration in a virtual material



Matrix thickness profile



CVI modeling : Summary

Numerical tools & strategy

- Two distinct numerical methods, specific to micro & macro scales, were chained together
- Work on 3D images (X-ray CMT scans, or virtual)

Comparison of the infiltrability of SiC_f/SiC_{SIP} preforms

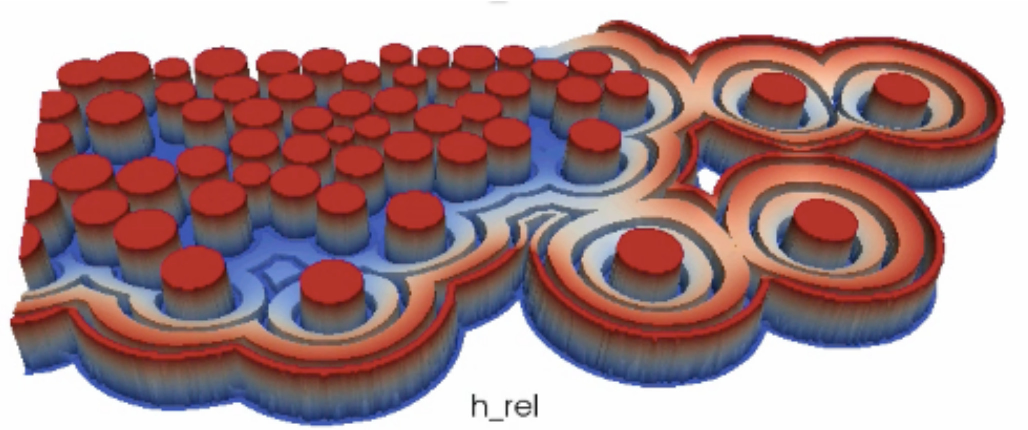
- Comparison of effective diffusivity, reactivity and microscale geometrical parameters
- Evidence of their effect on the macrosale infiltrability of these preforms

Insertion in a virtual material toolbox

- Computation at various scales
- A design tool from weaving to the final matrix
- Transferred to the industry

Part 4

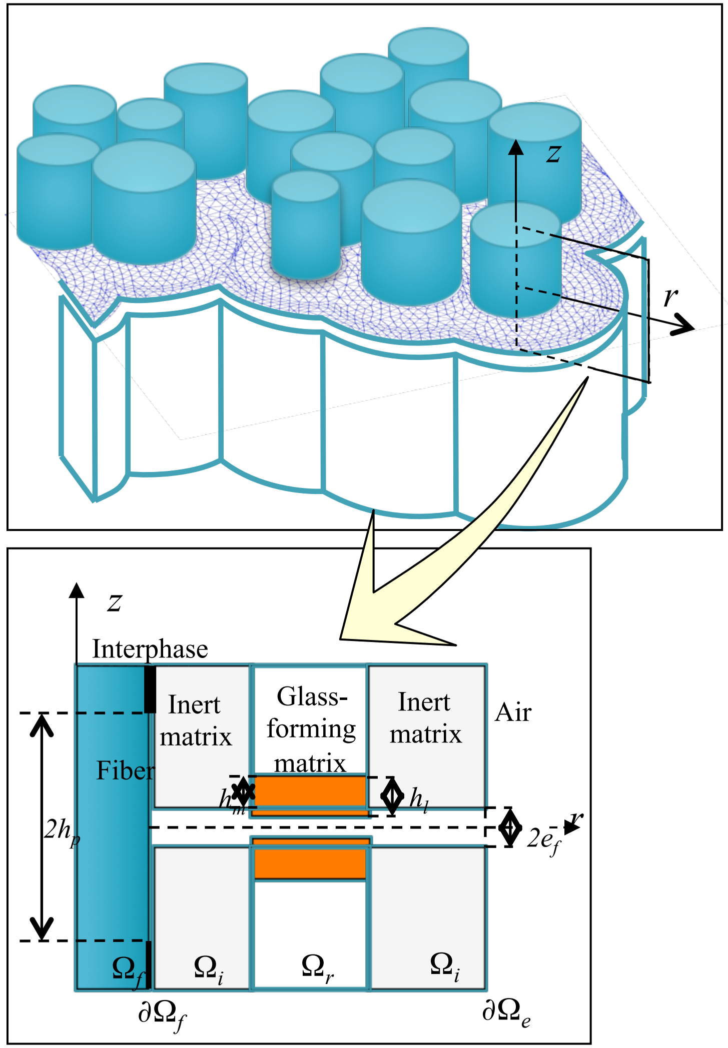
MODELLING OXIDATION AND SELF-HEALING



Problem assumptions

Transverse crack image-based modeling :

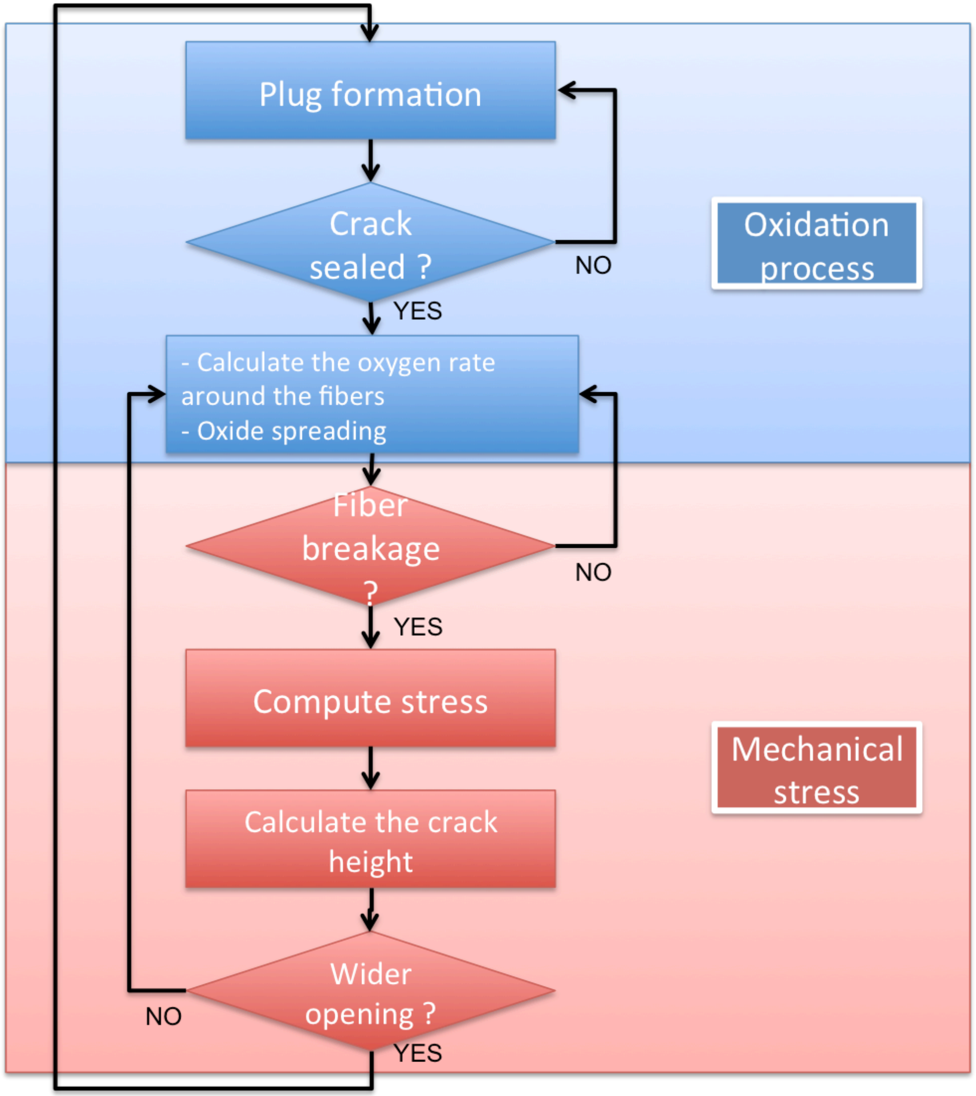
- Crack width is a function of 2D space
- Diffusion of oxygen as gas and/or dissolved species in liquid
- Liquid height is a function of space
- Evolution equation for interphase consumed height
- Liquid spreading
- Volatilization is not (yet) accounted for



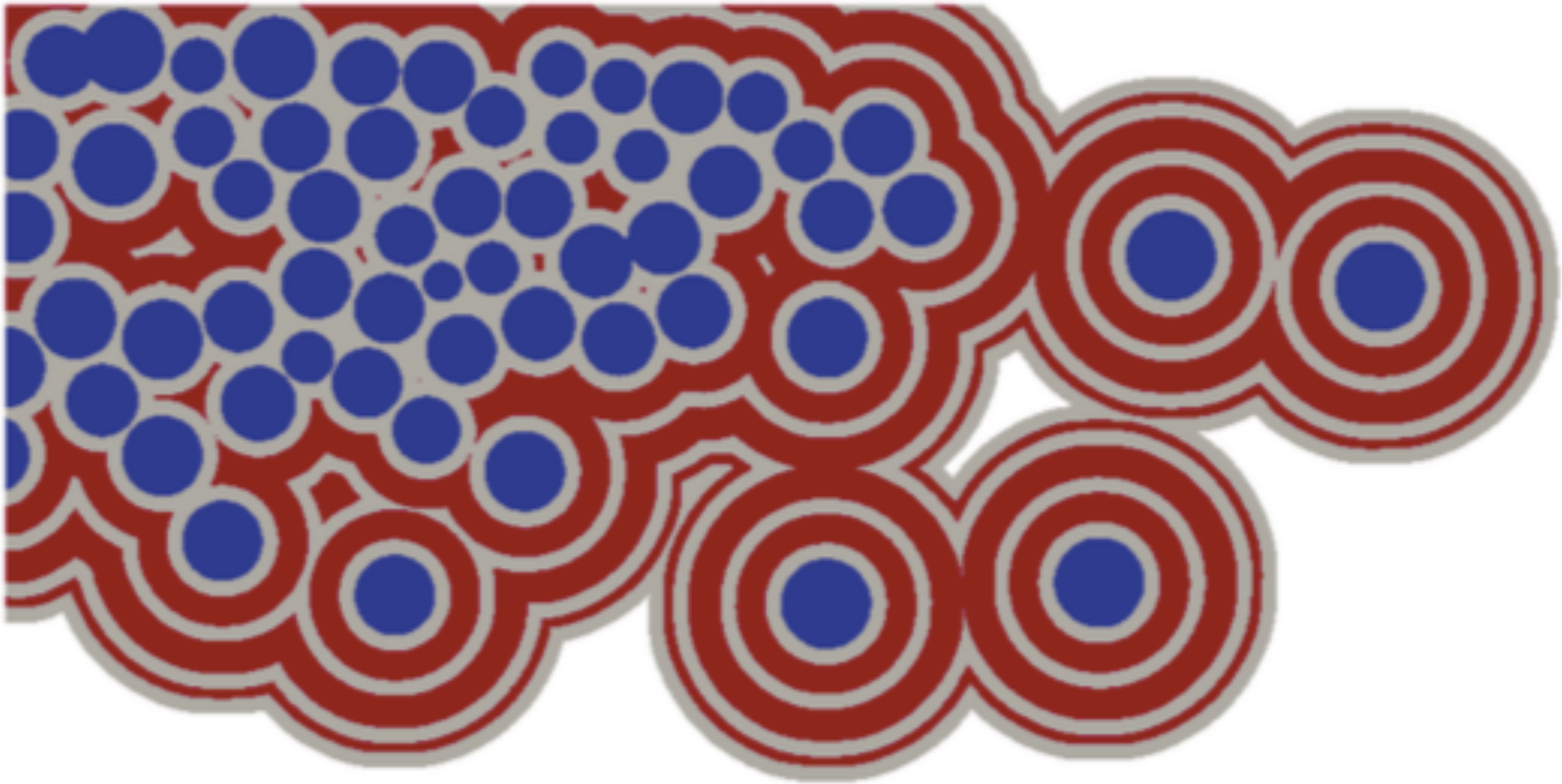
Mechanical behavior :

- Weibull distribution
- SCG law ➔ strength decrease

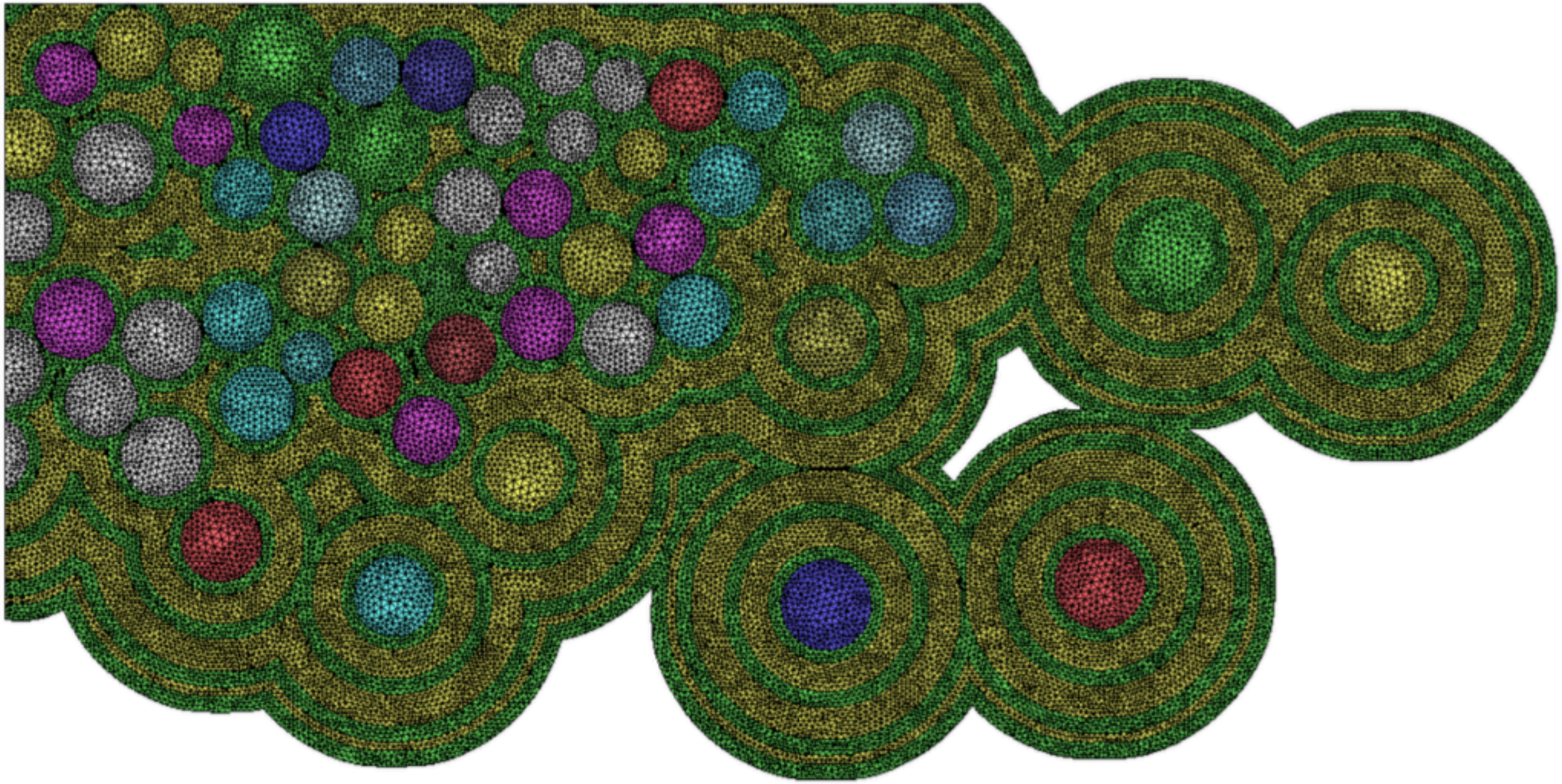
Lifetime computation algorithm



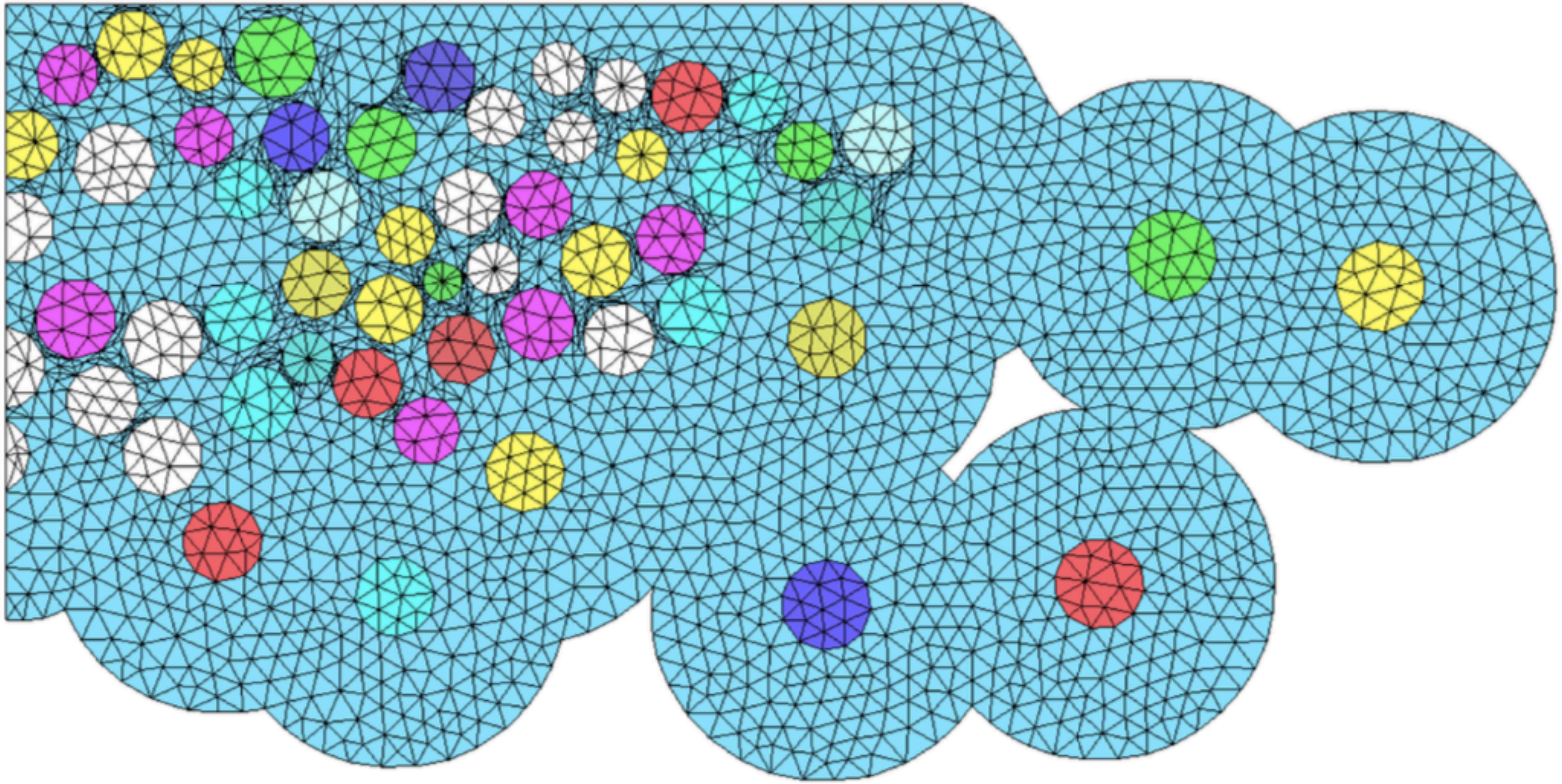
Resolution domain: minicomposite

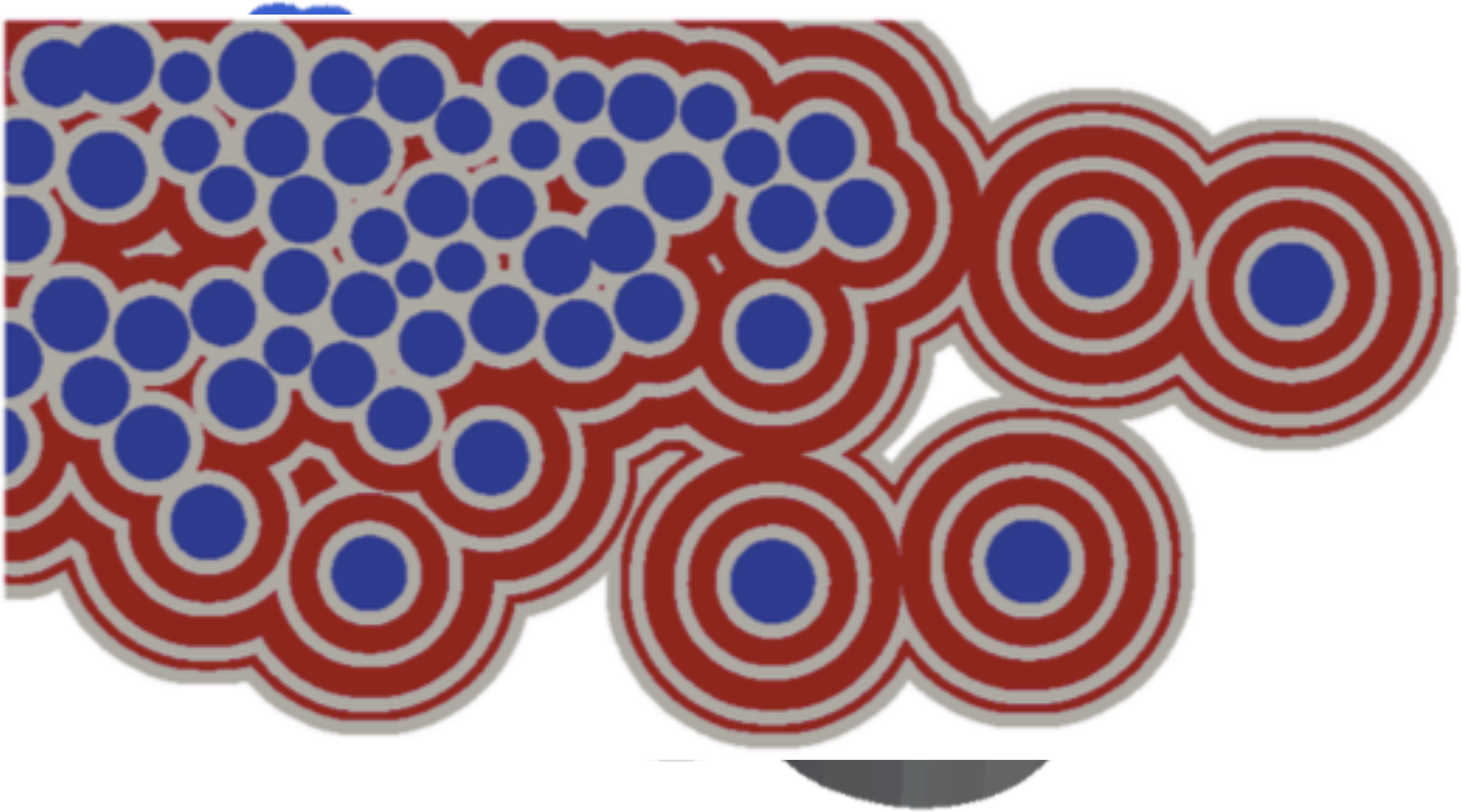


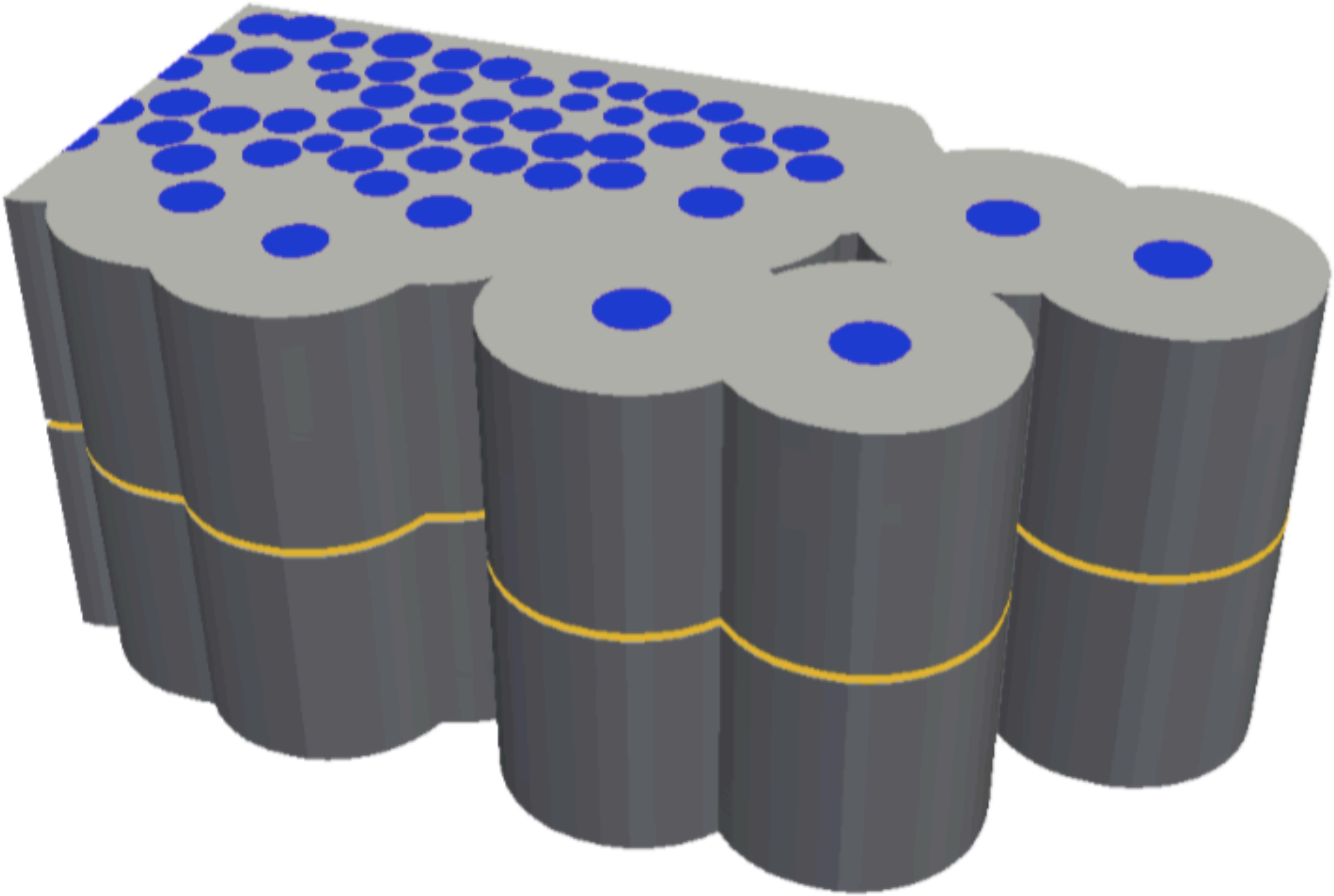
Fine mesh for physico-chemistry

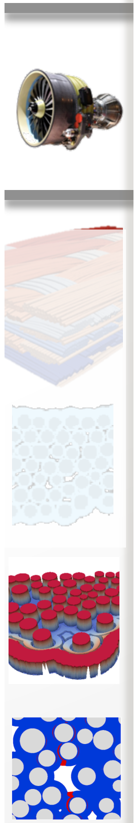


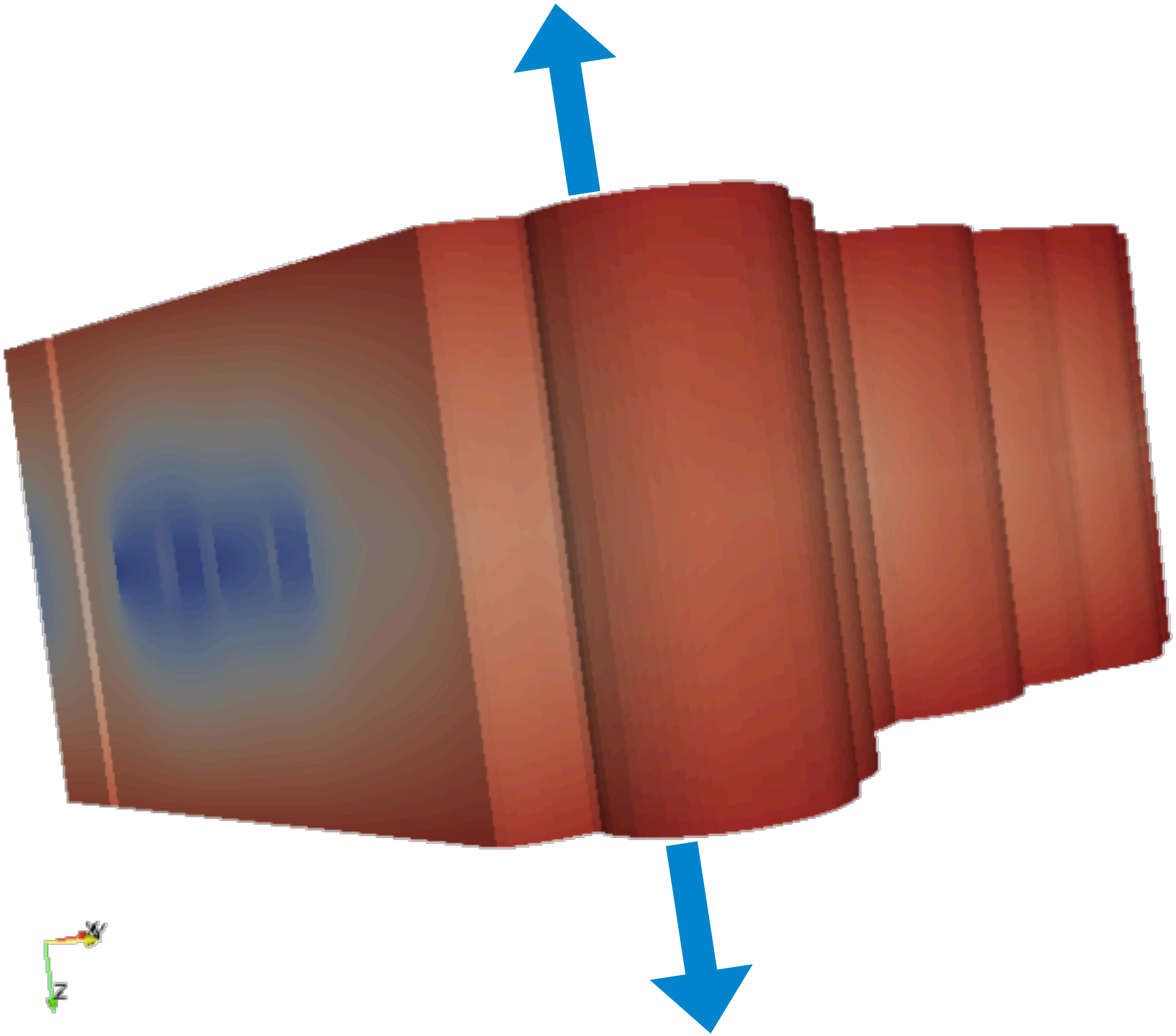
Coarse mesh for mechanics

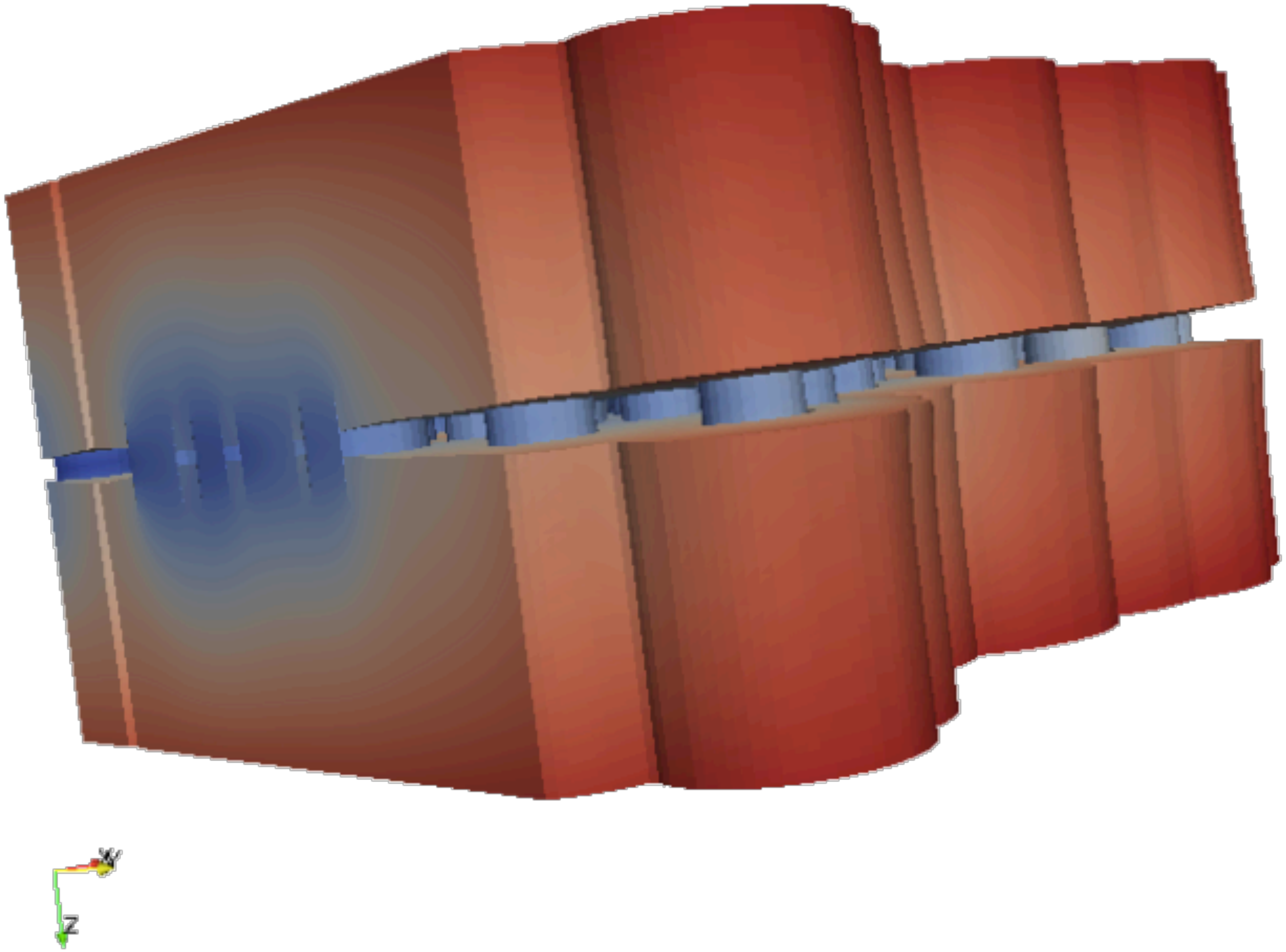




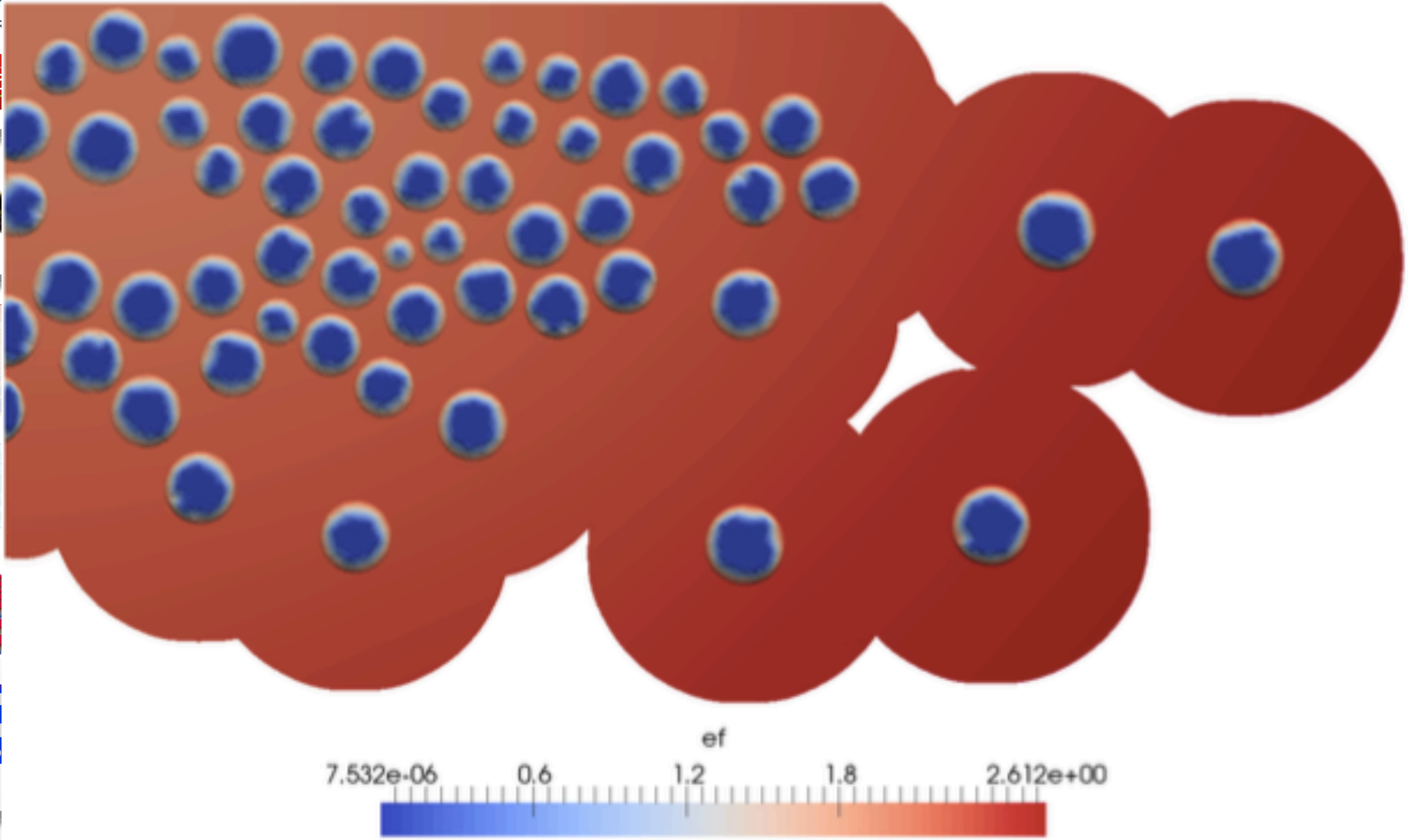


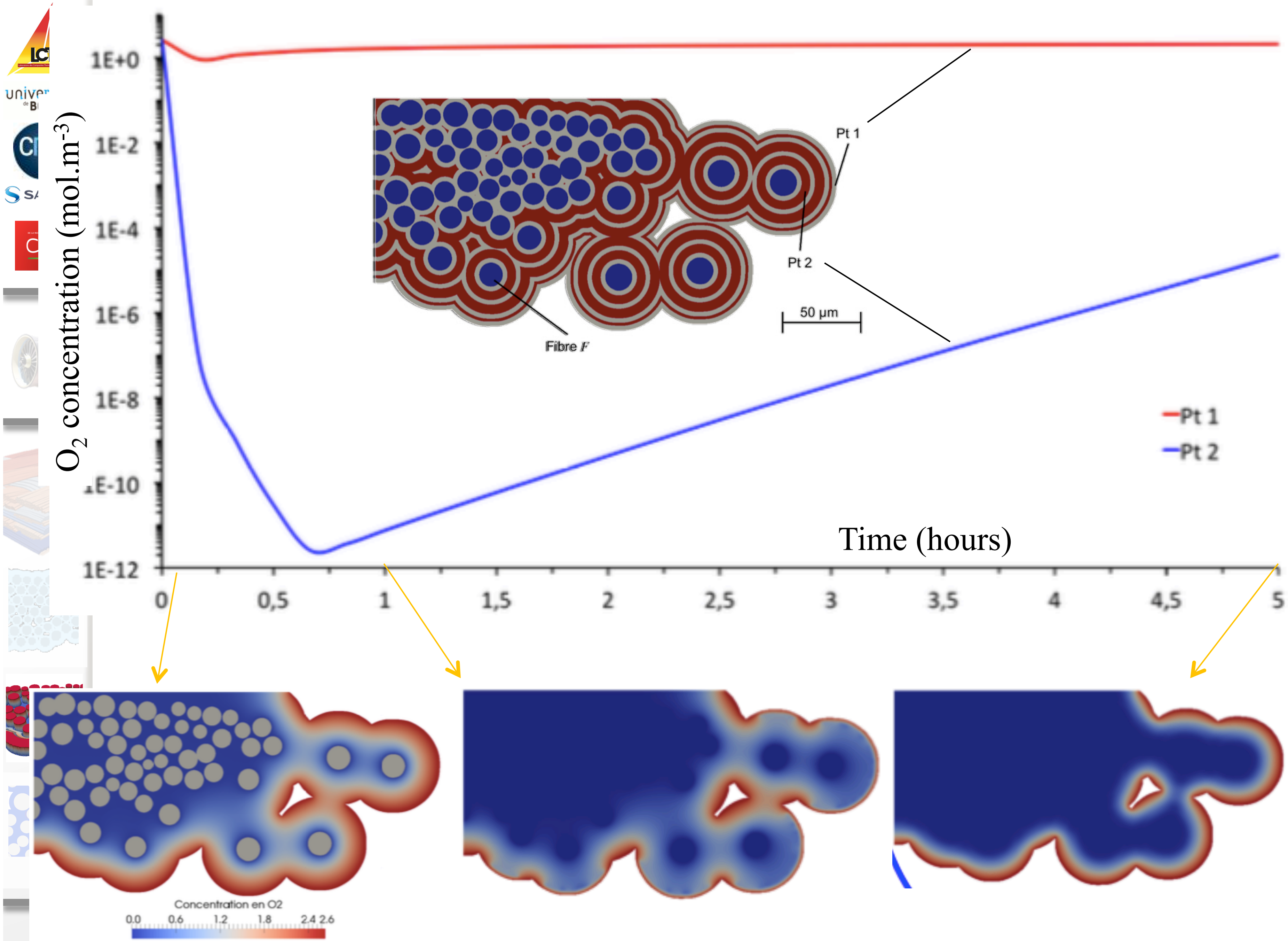



Z



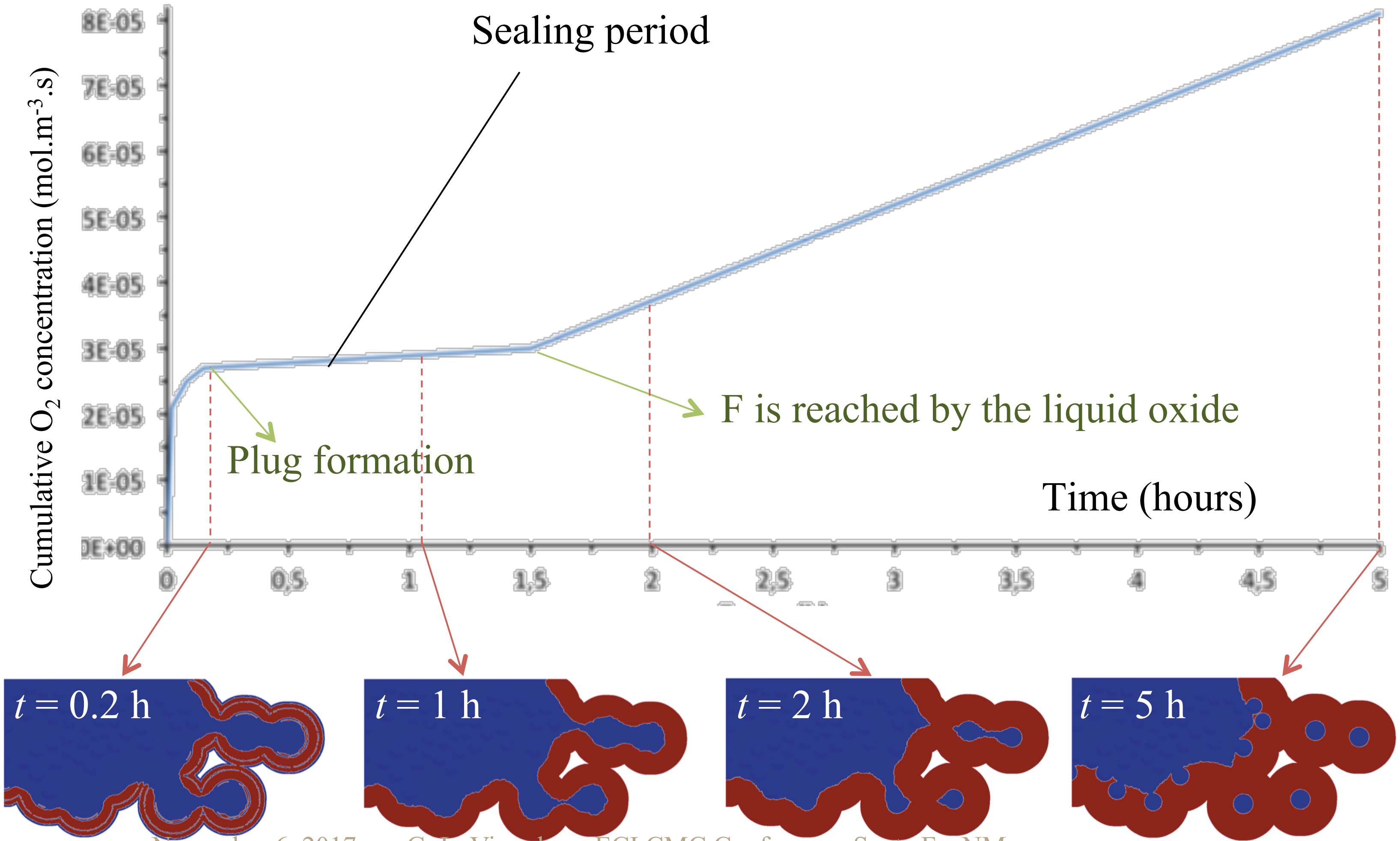
Variable crack width



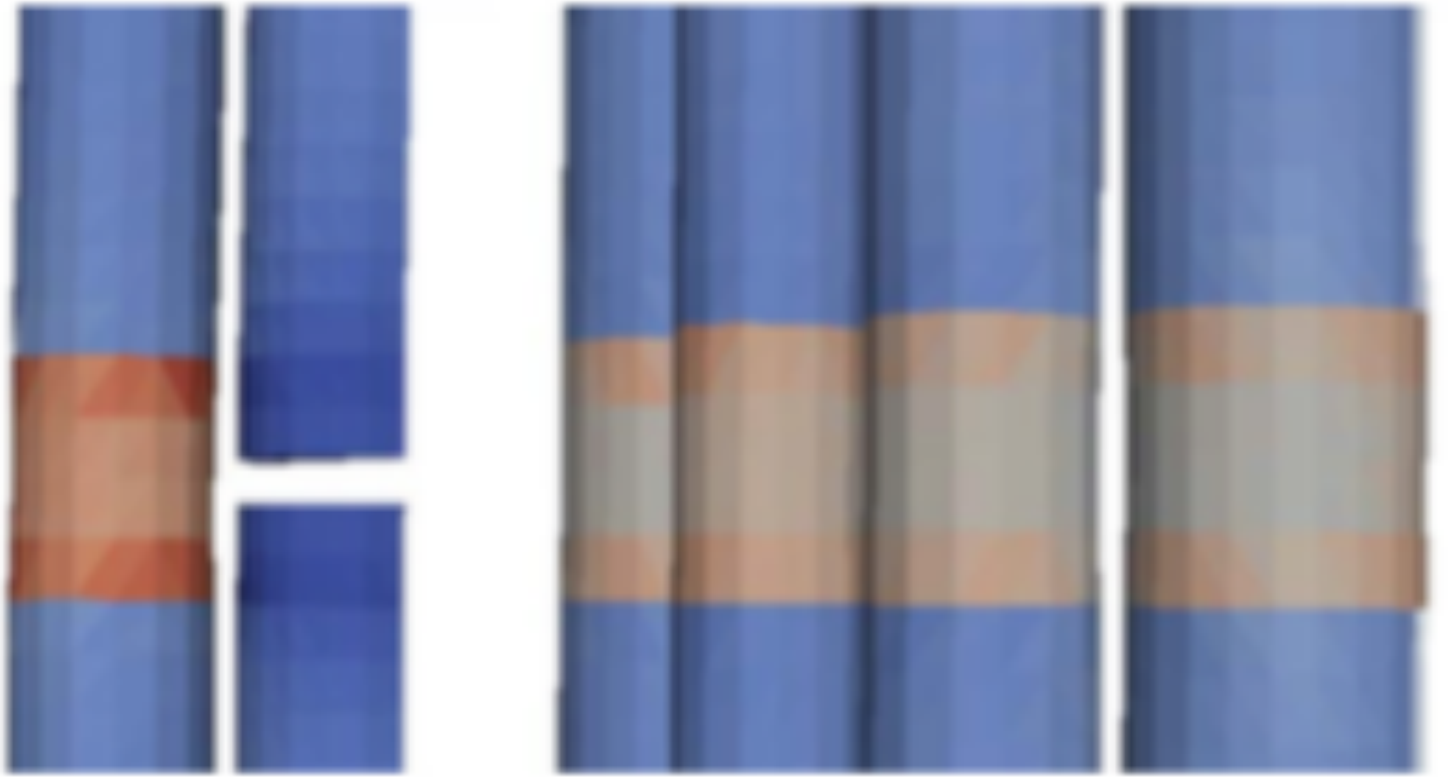


O$_2$ concentration (mol.m^{-3})
1E+0
1E-2
1E-4
1E-6
1E-8
1E-10
1E-12
0
0,5
1
1,5
2
2,5
3
3,5
4
4,5
5
Time (hours)
Pt 1
Pt 2
Fibre F
50 µm
Concentration en O2
0.0 0.6 1.2 1.8 2.4 2.6

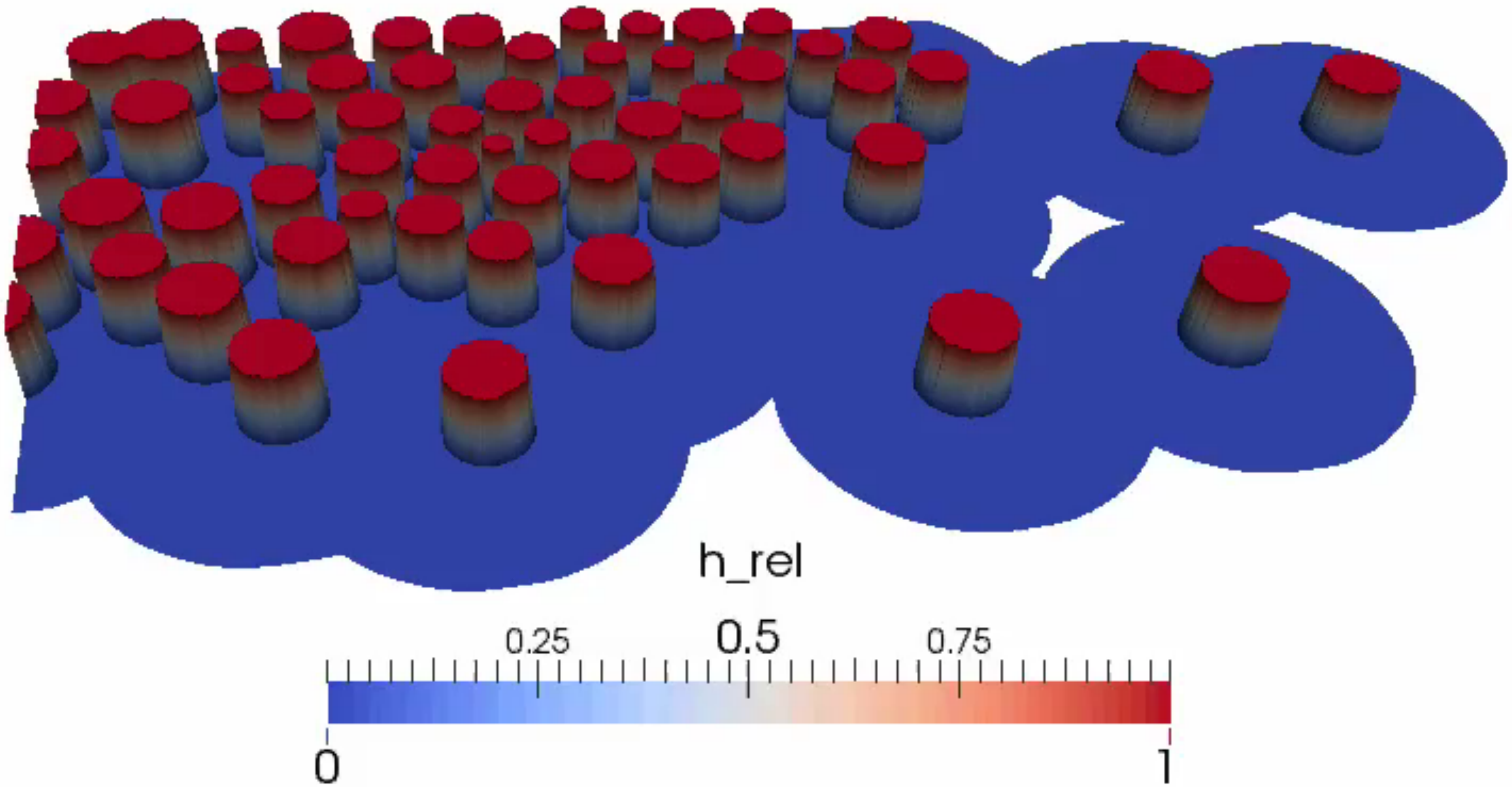
Sealing behavior



Fiber failure & local reloading

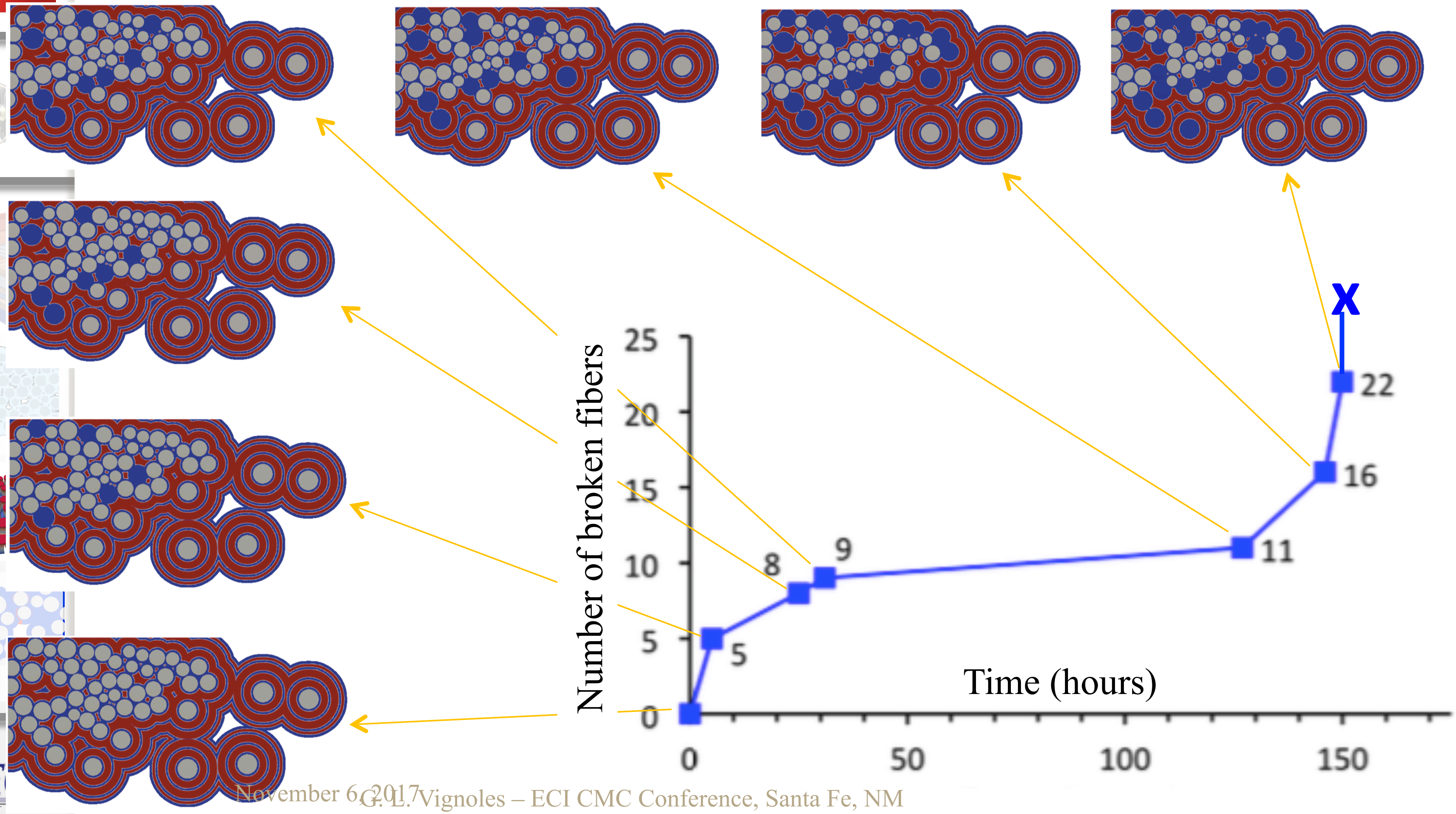


Meso-model of oxidation, healing, partial fiber breakage and re-healing

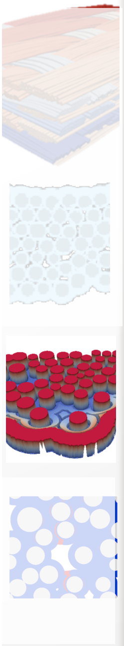


Crack oxidation and sealing → Breakage: crack reopening → Oxidation restarts

Progressive failure of the bundle



SH-CMC simulation: Summary



Numerical tools & strategy

- Image-based approach
- Multiphysics code
- Gives convincing scenarii for bundle weakening & failure

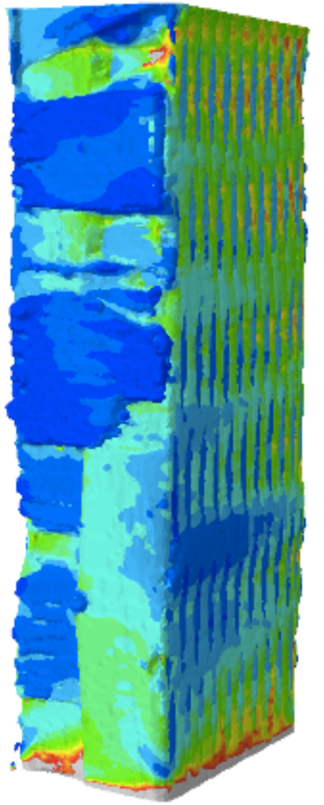
Outlook

- Perform a statistical study
- Extension to longitudinal cracks
- Integration in crack networks

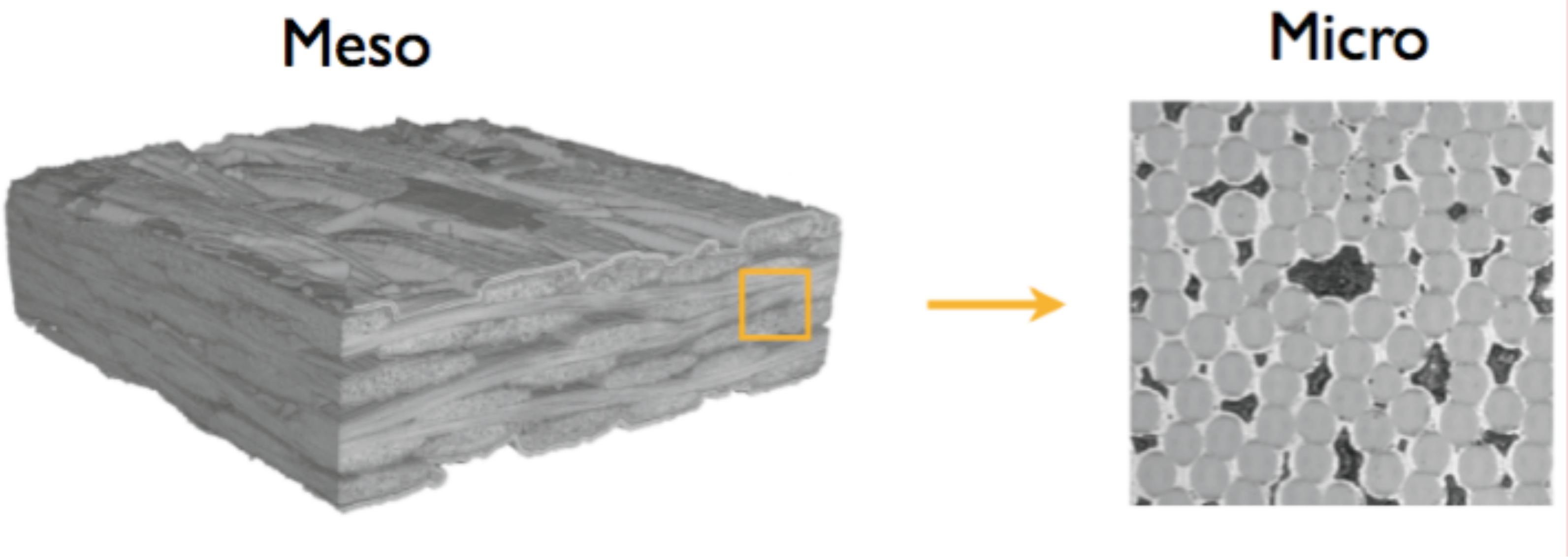
New funding obtained !

Part 5

MODELLING OF MECHANICAL BEHAVIOR



2-scale mechanical computations

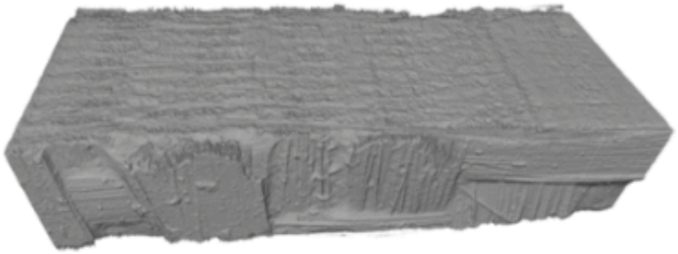


Non-linear mechanics due to multicracking:

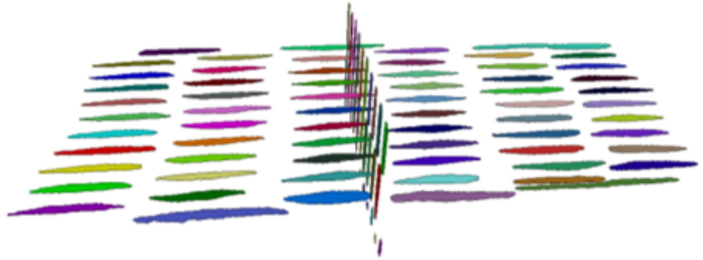
→ Localization of stress concentrations
→ Introduction of cracks in FE meshes
→ How to get a good FE mesh, by the way ?

Yarn-scale FE mesh generation

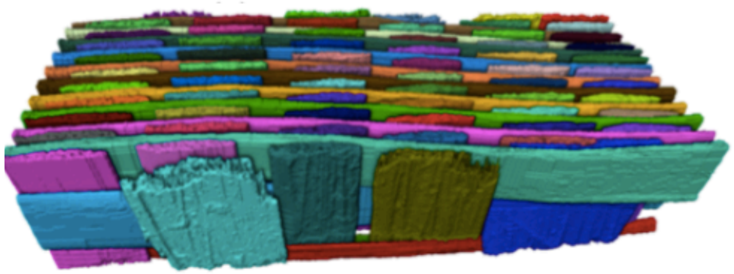
V. Mazars, O. Caty, G. Couegnat, A. Bouterf, S. Roux, S. Denneulin, J. Pailhes, G. L.Vignoles, *Acta Materialia*, **140**, 130–139 (2017).



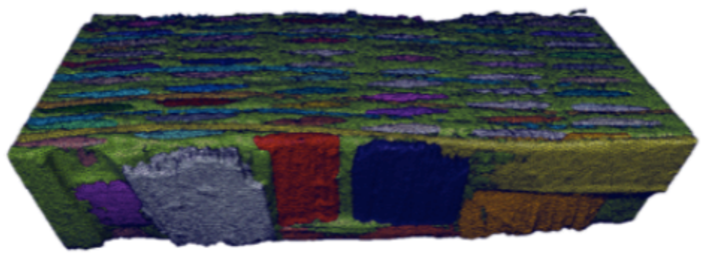
µ-CT scan



Manual contouring on 2 transverse slices



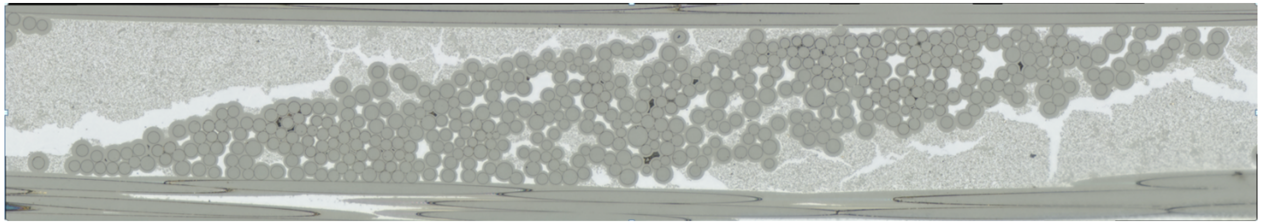
Orientation detection
& segmentation



Marching-cube &
simplification
+ Volume meshing

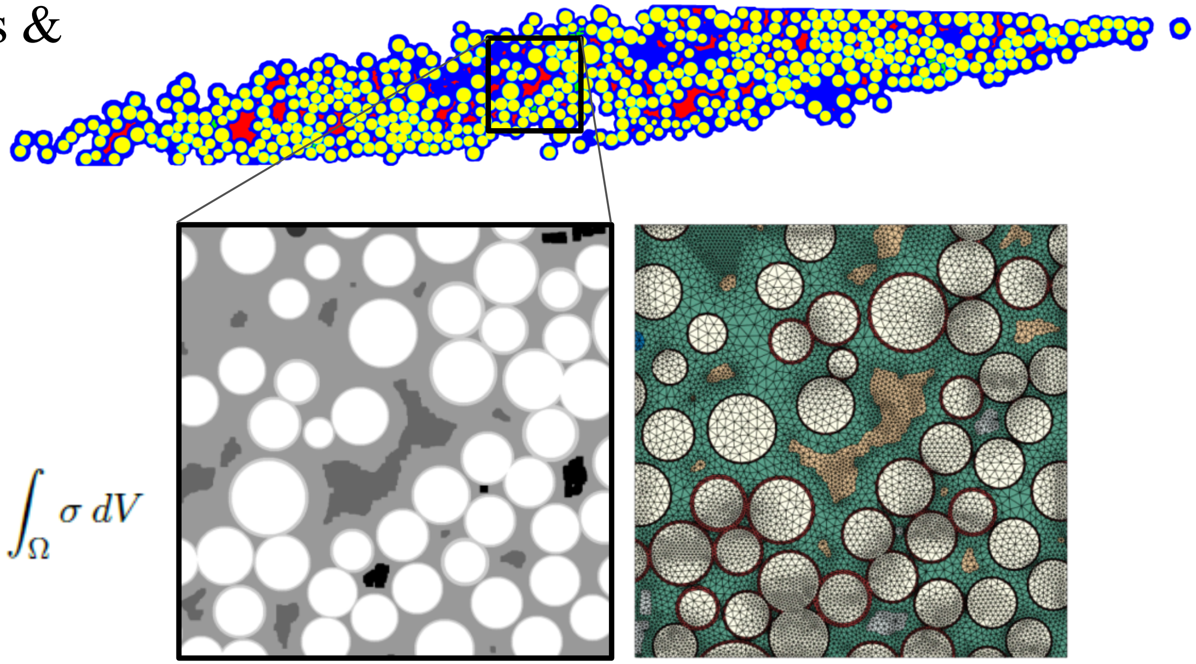
Fiber-scale FE mesh generation & computations

Micrographs



Segmentation of fibers & matrix

2D Meshing



Numerical homogenization

$$\langle \epsilon \rangle = \frac{1}{V_\Omega} \int_\Omega \epsilon \, dV, \quad \langle \sigma \rangle = \frac{1}{V_\Omega} \int_\Omega \sigma \, dV$$

$$\langle \sigma \rangle = C^{app} : \langle \epsilon \rangle$$

The transverse isotropic properties are transferred to yarns

$$\begin{pmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ \sqrt{2}\epsilon_{23} \\ \sqrt{2}\epsilon_{13} \\ \sqrt{2}\epsilon_{12} \end{pmatrix} = \begin{pmatrix} \frac{1}{E_1} & -\frac{\nu_{12}}{E_1} & -\frac{\nu_{13}}{E_1} & 0 & 0 & 0 \\ -\frac{\nu_{21}}{E_2} & \frac{1}{E_2} & -\frac{\nu_{23}}{E_2} & 0 & 0 & 0 \\ -\frac{\nu_{31}}{E_3} & -\frac{\nu_{32}}{E_3} & \frac{1}{E_3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2G_{23}} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2G_{13}} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2G_{12}} \end{pmatrix} \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sqrt{2}\sigma_{23} \\ \sqrt{2}\sigma_{13} \\ \sqrt{2}\sigma_{12} \end{pmatrix}$$

Tensile test under µ-CT

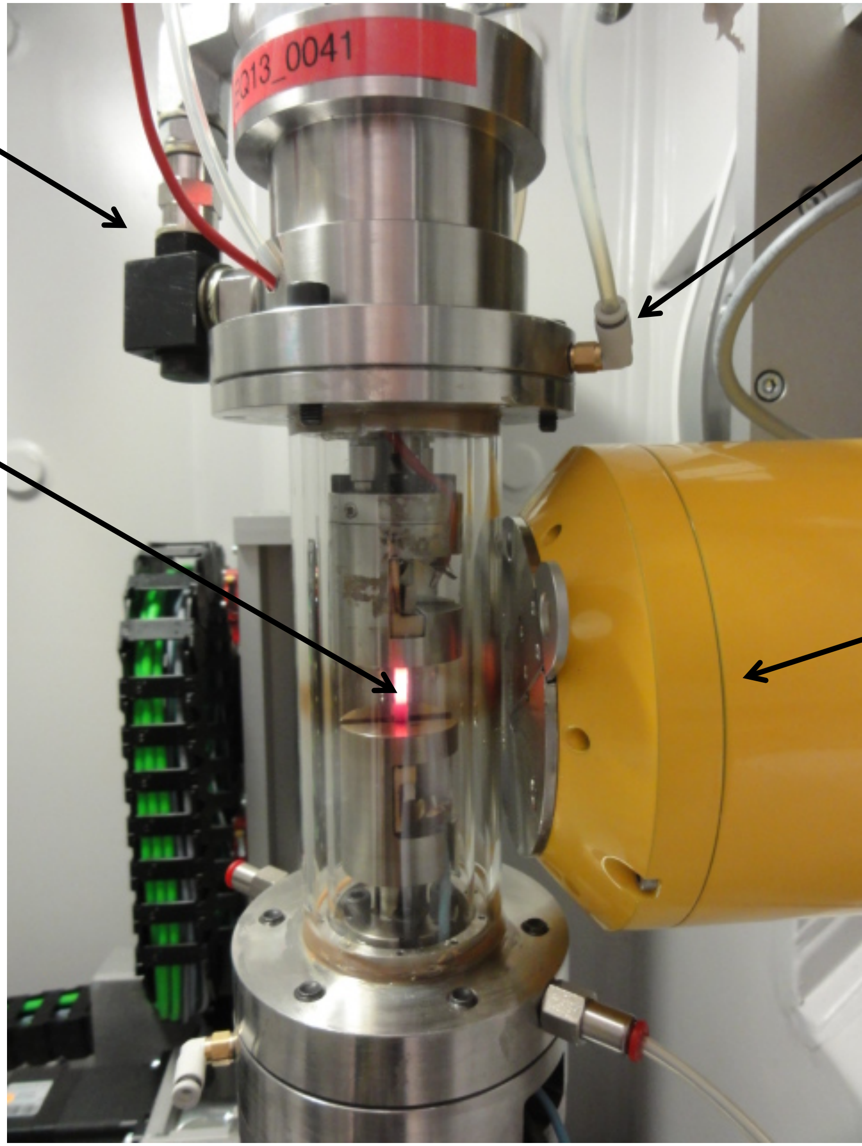
V. Mazars et al., *Acta Materialia*, **140**, 130–139 (2017).

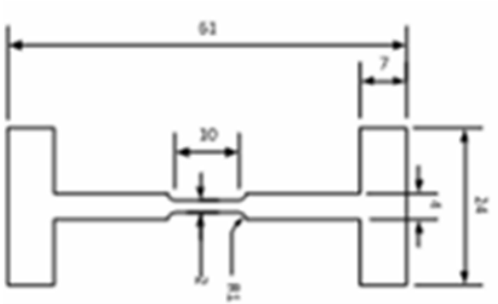
Hydraulic load
5000N

Joule heating

Air cooling

X-ray source
(GE Vtom X,
Placamat)



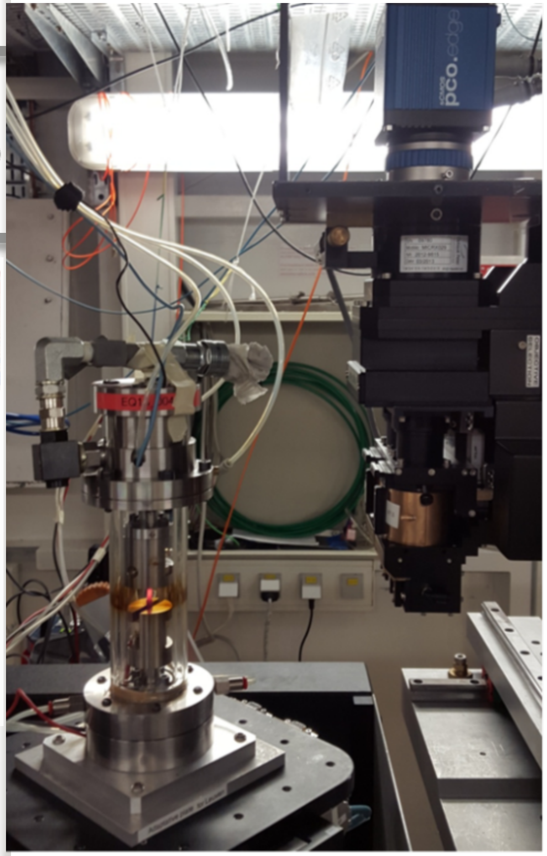


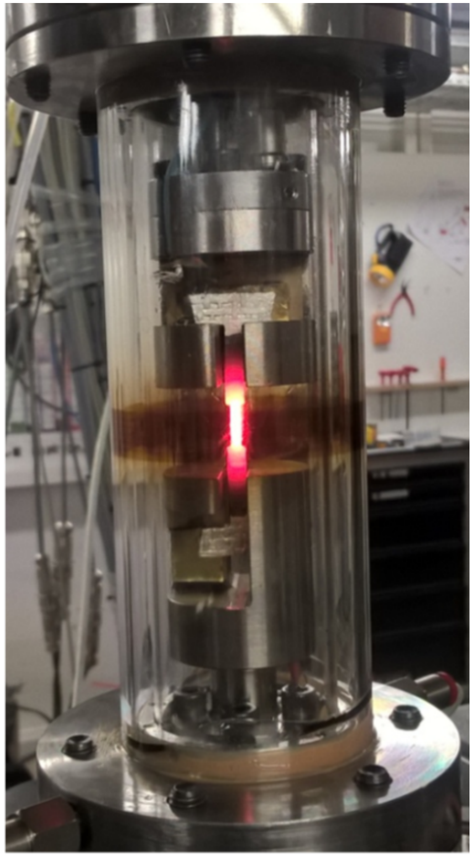
SiC/SiC MI samples
Section : 2x3 mm²
Gauge length: 10 mm

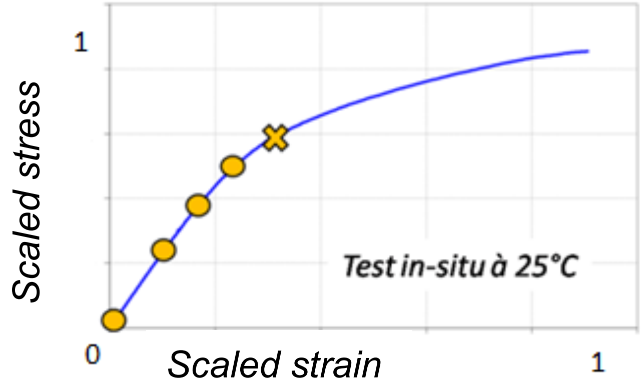
In-situ testing

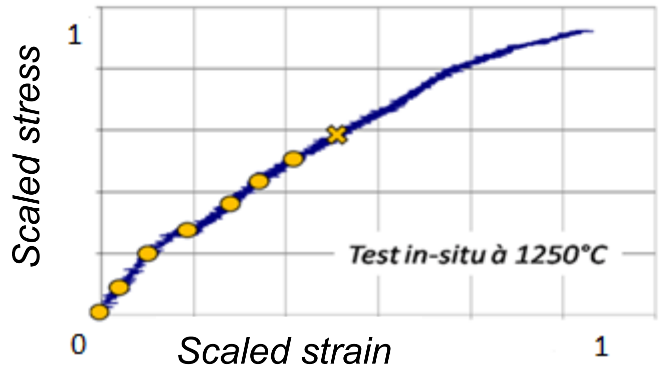
V. Mazars et al., *Acta Materialia*, **140**, 130–139 (2017).

ID19 beamline ESRF
Resolution : 1 µm









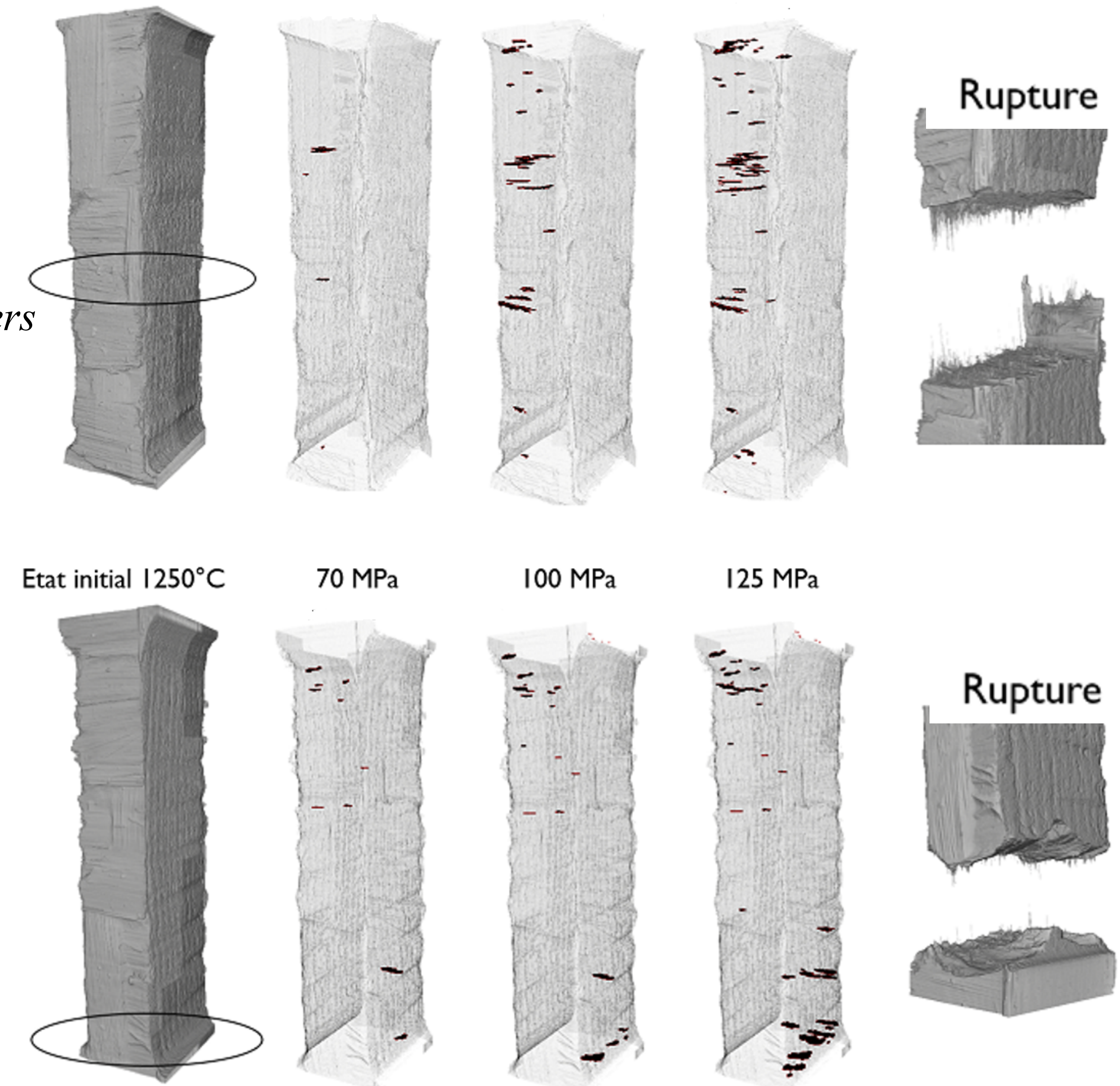
Crack detection by image analysis

V. Mazars et al., *Acta Materialia*, **140**, 130–139 (2017).

Procedure :

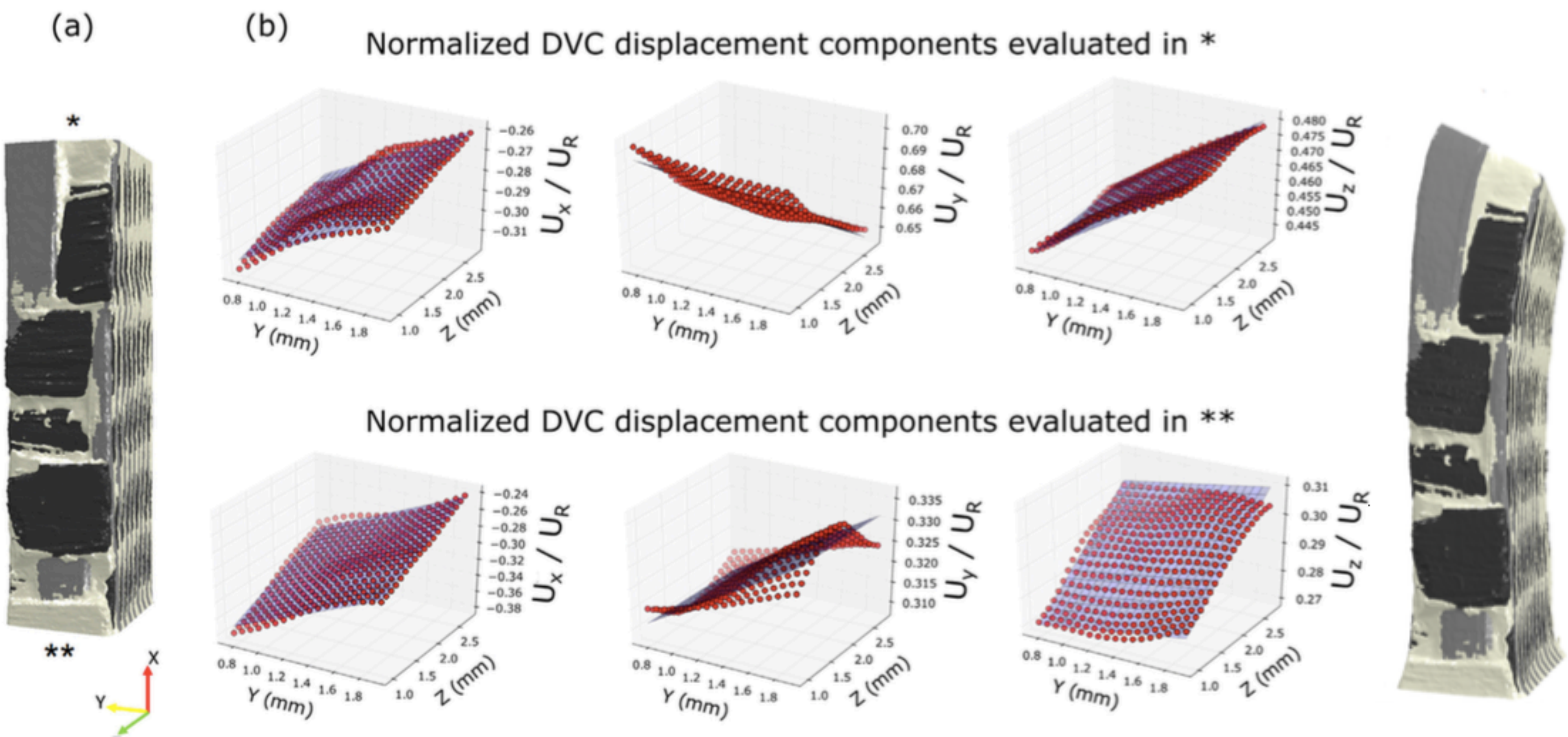
i. Scaling factor : 2
ii. RBM correction (Avizo ®)
iii. Difference fields
iv. Morphological filters
v. Manual control

- Cracks from surface, perpendicular to tensile load
- Initiation & propagation in pre-damaged zones



Retrieval of boundary conditions by DVC

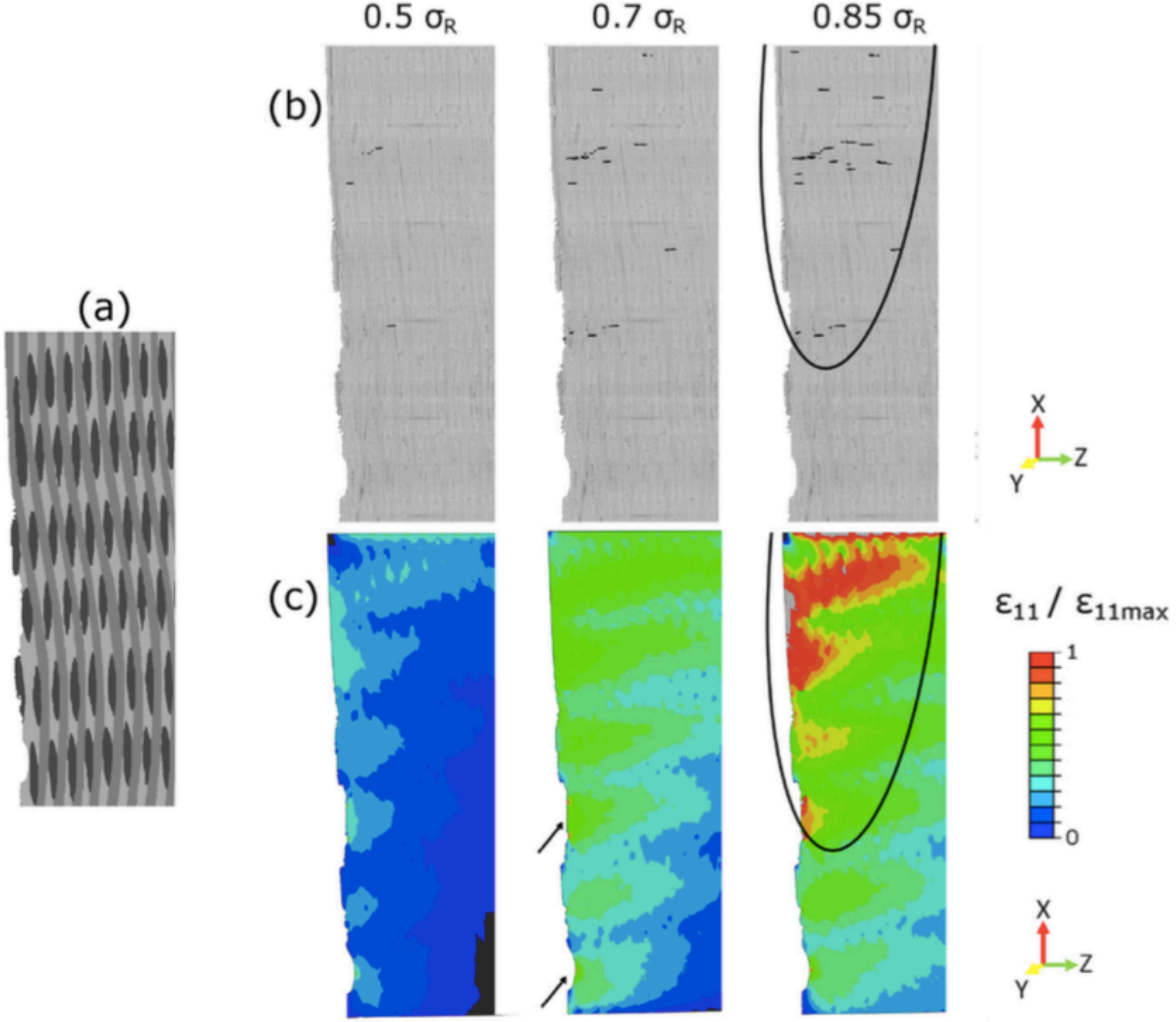
V. Mazars et al., *Acta Materialia*, **140**, 130–139 (2017).

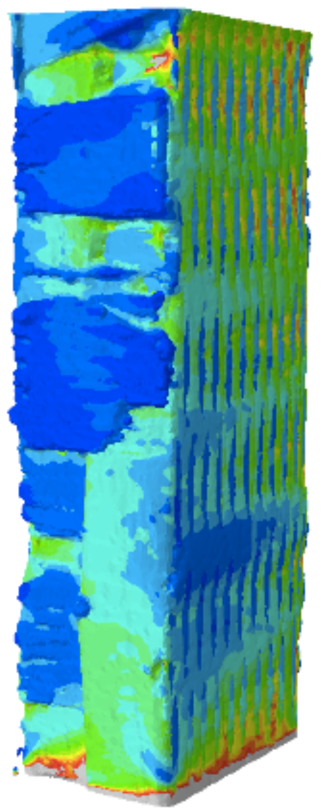


Actual strain

Elastic computations

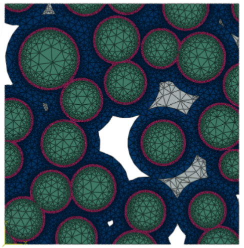
V. Mazars et al., *Acta Materialia*, **140**, 130–139 (2017).



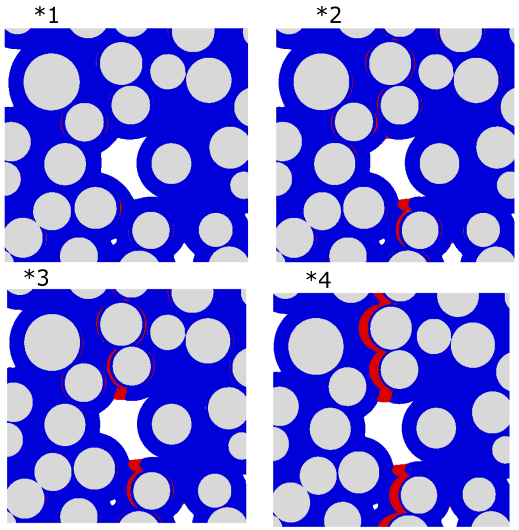


Cracks & overloads coincide

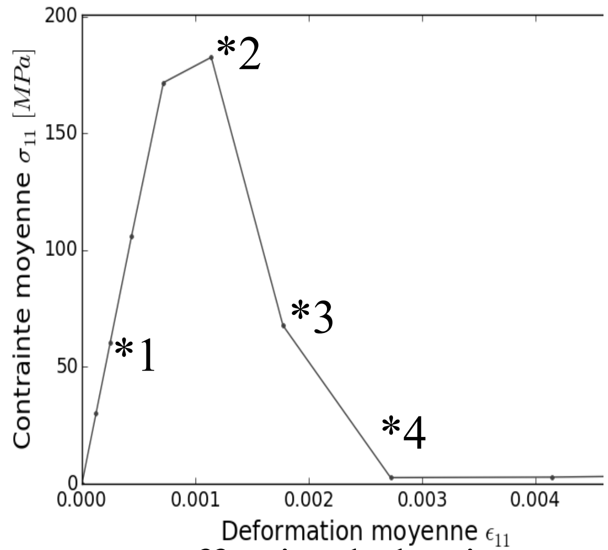
Multi-scale damage modeling



Micro cells



Cohesive interface, brittle matrix



Effective behavior

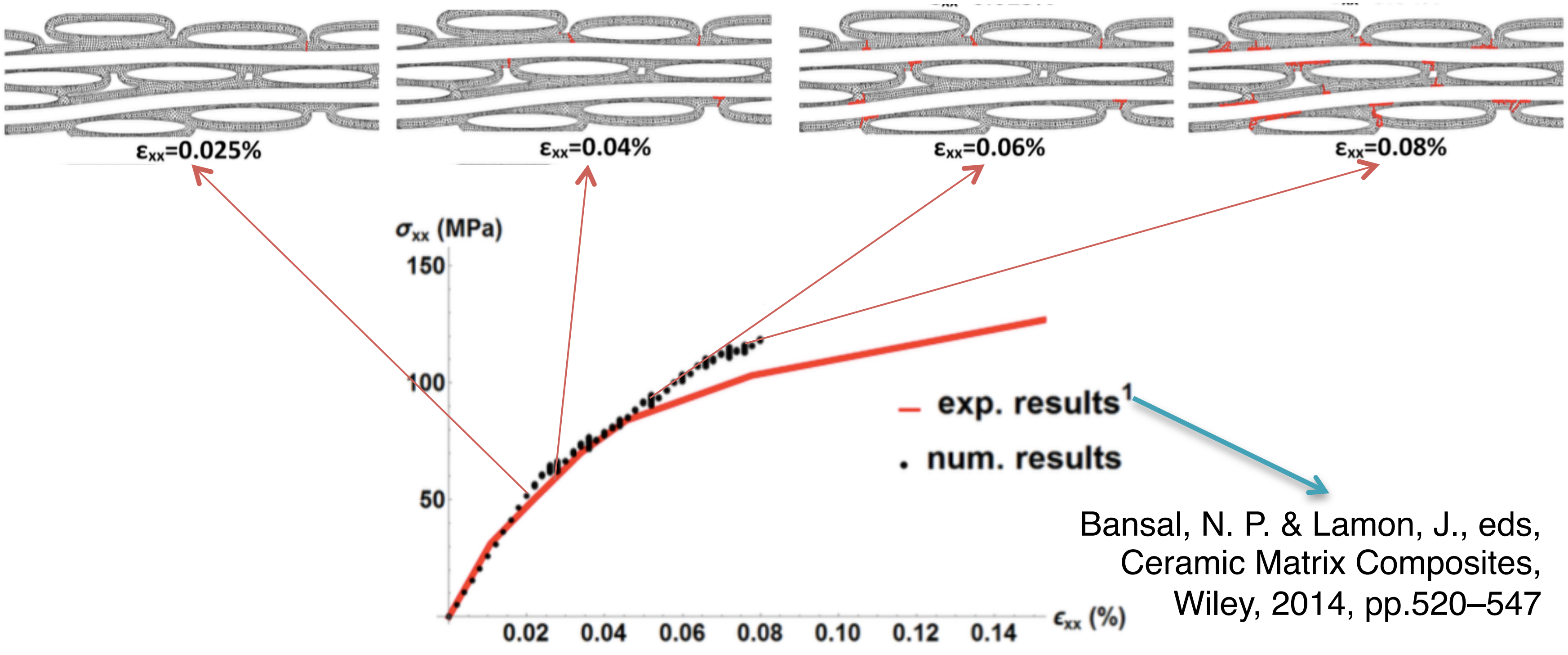
Transposition of stiffness abatement

Mesoscale damage computation

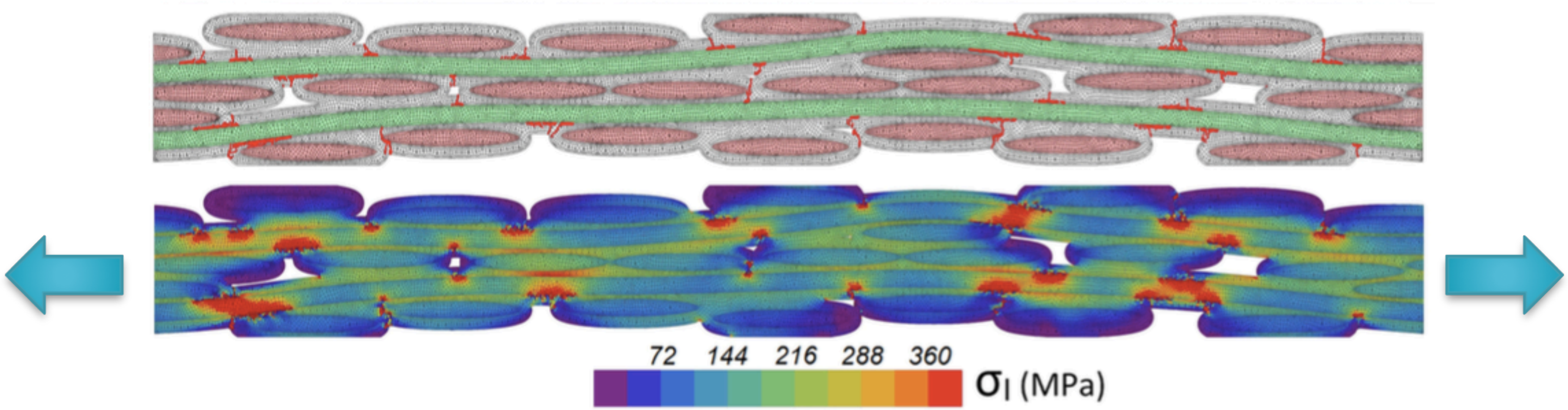
… IN PROGRESS …

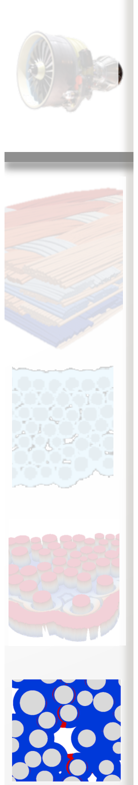
A-FEM method

S. Essongue, PhD dissertation, U. Bordeaux (2016)



Bansal, N. P. & Lamon, J., eds, Ceramic Matrix Composites, Wiley, 2014, pp.520–547





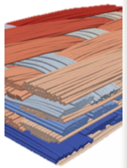
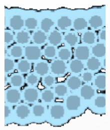
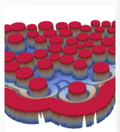
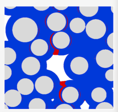
Mechanics: Summary & Outlook

Numerical tools & strategy

- From images to FE meshes
- Multi-scale strategy
- Experimental verification vs. μ-CT :
    - Role of DVC in crack detection & BC retrieval
    - Cracks match overloaded areas (yarns crossings)

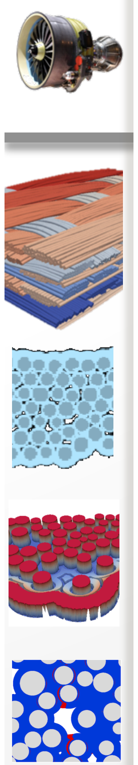
Outlook

- FE meshing procedure development still under way
- Failure mechanics under way …

General conclusion

- Multiscale /multiphysics approaches
- Dialog between experiments & modeling
- Multidisciplinary work :
  - Structural characterization (image acquisition ; properties)
  - Image processing (analysis ; synthesis)
  - Physico-chemical (« multi-physics ») modeling
  - Numerical tools (meshes, solvers, etc …)
- A broad field of possibilities : every material, every application brings its « own » physico-chemistry
- From basic science to application and innovation



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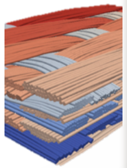

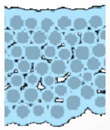

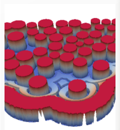

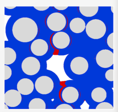

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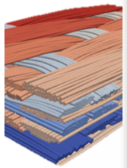
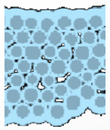
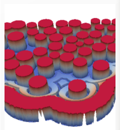
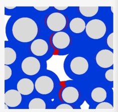
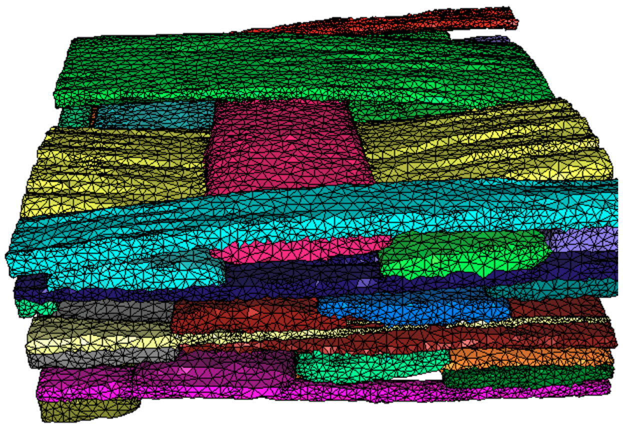
New !











¡ Gracias por su atención !

¿ Preguntas ?

HT-CMC/10th
Bordeaux 22-27 SEPT. 2019
10th International Conference on High Temperature Ceramic Matrix Composites
ht-cmc10.org

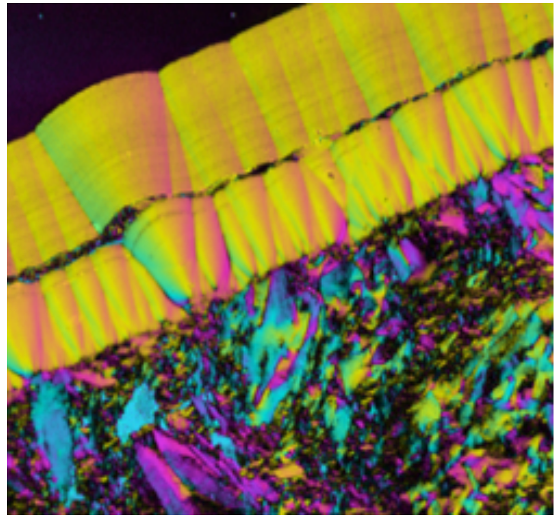
Workshop announcement

Bulk Carbon Materials (composites, fibers, films, foams, porous carbons, etc.):

Relationships between processing conditions and the resulting structure, texture, and properties

a.k.a. "the 3rd PyroMaN workshop"

Madrid, Spain **June 29-30, 2018**



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