

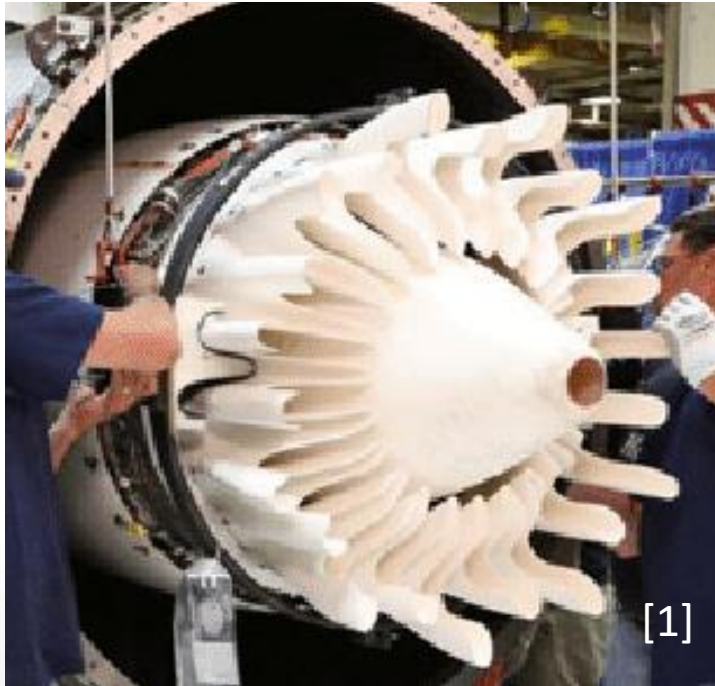
# A numerical method to simulate the intra-tows mechanical behaviour of oxide/oxide CMCs: coupling of a lattice with a finite element continuum

Thierry Canet, Thierry Cutard, Gilles Dusserre

ECERS 2023 symposium S4

## Summary :

- **Context and issues**
- Presentation of the calculation method by lattice of connectors and FEM coupling
- Presentation of the results
- Conclusion and outlooks



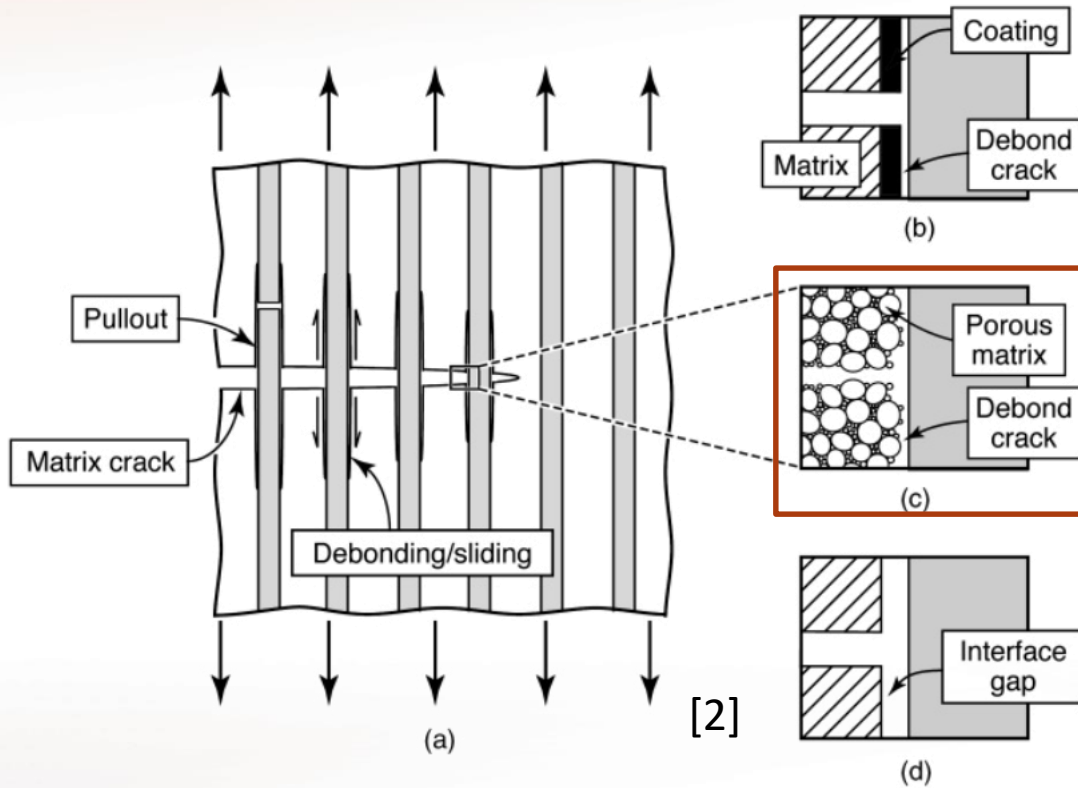
GE passport 20 nozzle rear body in CMC Alumina/Alumina

Porous ceramics have many applications, particularly as a matrix in oxide/oxide Ceramic Matrix Composites (CMC).

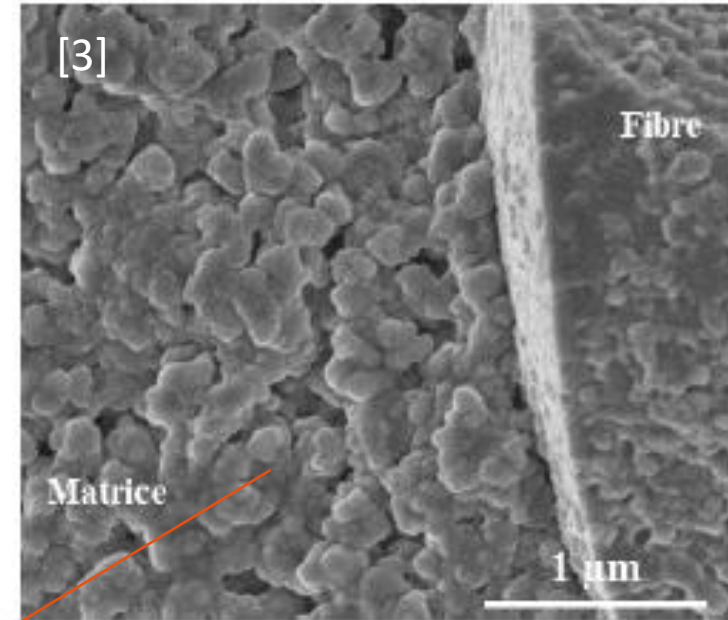
Such structures offer the following advantages :

- Good creep behaviour,
- Good oxidation resistance at high temperature,
- Better toughness than monolithic ceramics.

[1] : Walter Krenkel, Wiley-VCH Verlag GmbH&Co. KGaA. 2008.



CMC alumina/ alumina-silica



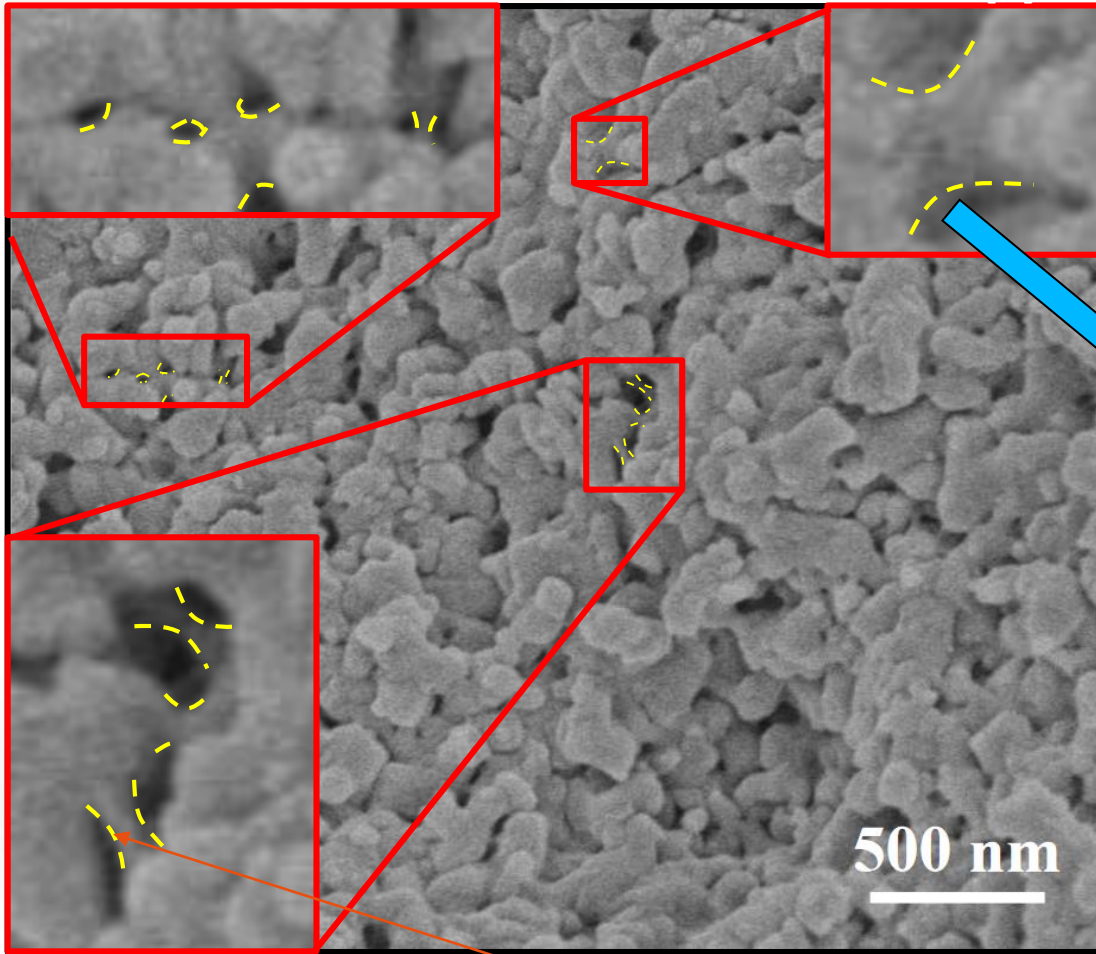
Optimising matrix porosity through process control

Modelling of the process/properties link.

[2] : F. W. Zok, *J American Ceramic Society*, vol. 89, n° 11, p. 3309-3324, nov. 2006

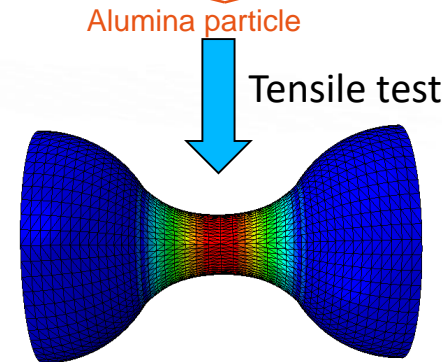
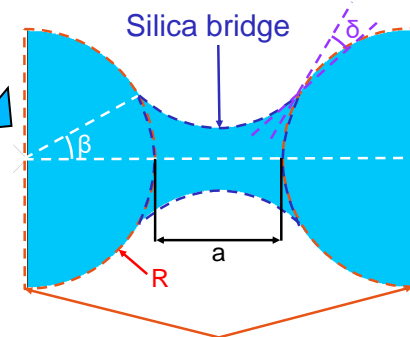
[3] : F. Boutenel, « Comportement d'une matrice alumine-silice au cours de l'élaboration de composites à matrice céramique oxyde/oxyde », thèse, novembre 2020.





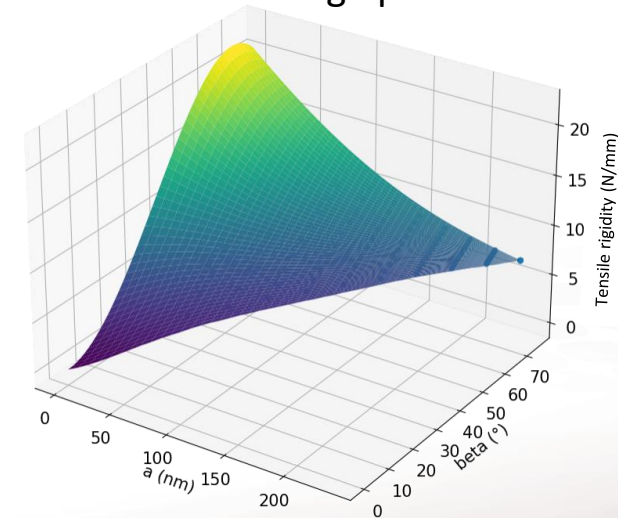
Silica bridge

Example of a microstructure of a porous alumina/silica matrix obtained by SEM (59%<sub>vol.</sub> Al<sub>2</sub>O<sub>3</sub>, 41%<sub>vol.</sub> SiO<sub>2</sub>).



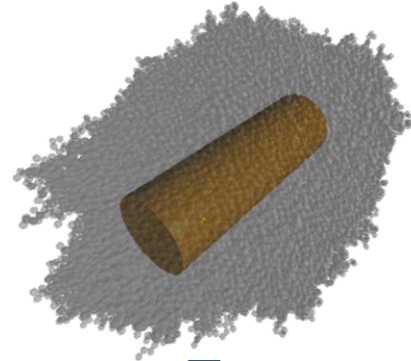
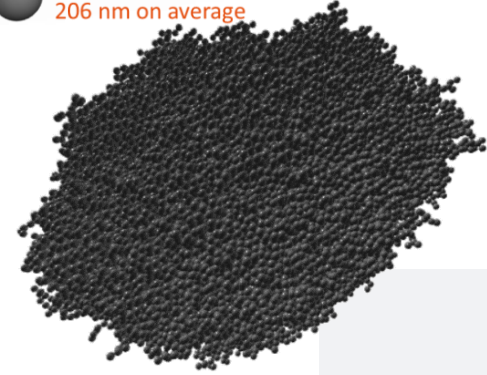
Alumina particle mean radius : 103 nm

Bezier surface of the tensile rigidity in function of bridge parameters



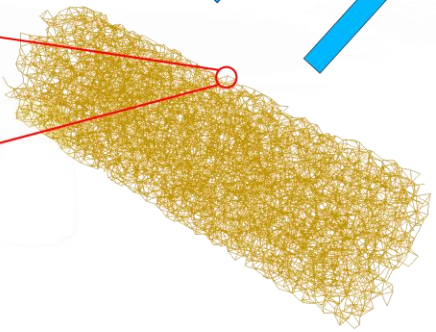
[3]: F. Boutenel, « Comportement d'une matrice alumine-silice au cours de l'élaboration de composites à matrice céramique oxyde/oxyde », novembre 2020

Alumina particle  
206 nm on average



Building the lattice of connector based on the volume of silica distributed on each particle

Modal Analysis

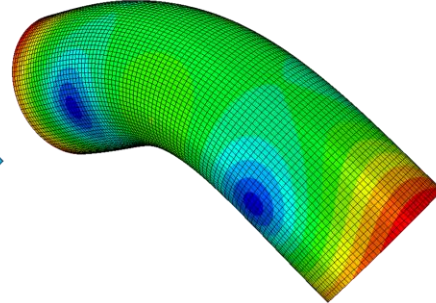


$f_{lattice} = 7414 \text{ Hz}$

Comparison  
Frequency relative deviation  $\approx 1,63\%$

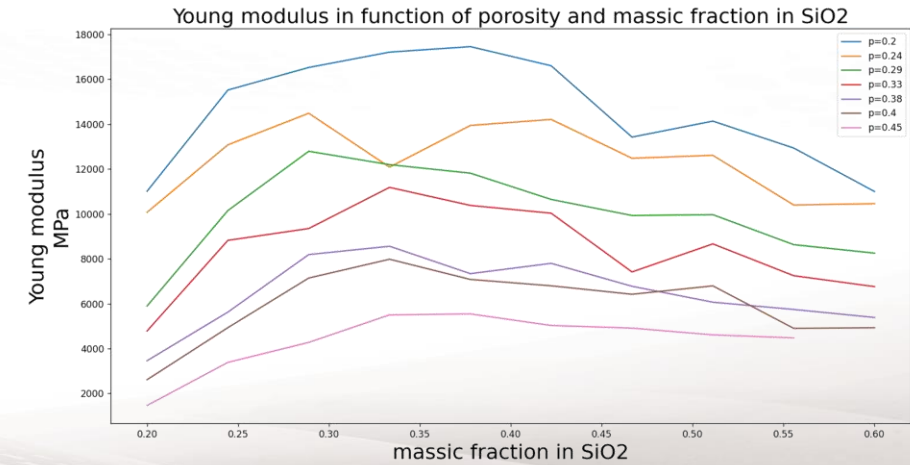


bending eigenmode  $\rightarrow E$   
Torsion eigenmode  $\rightarrow G$



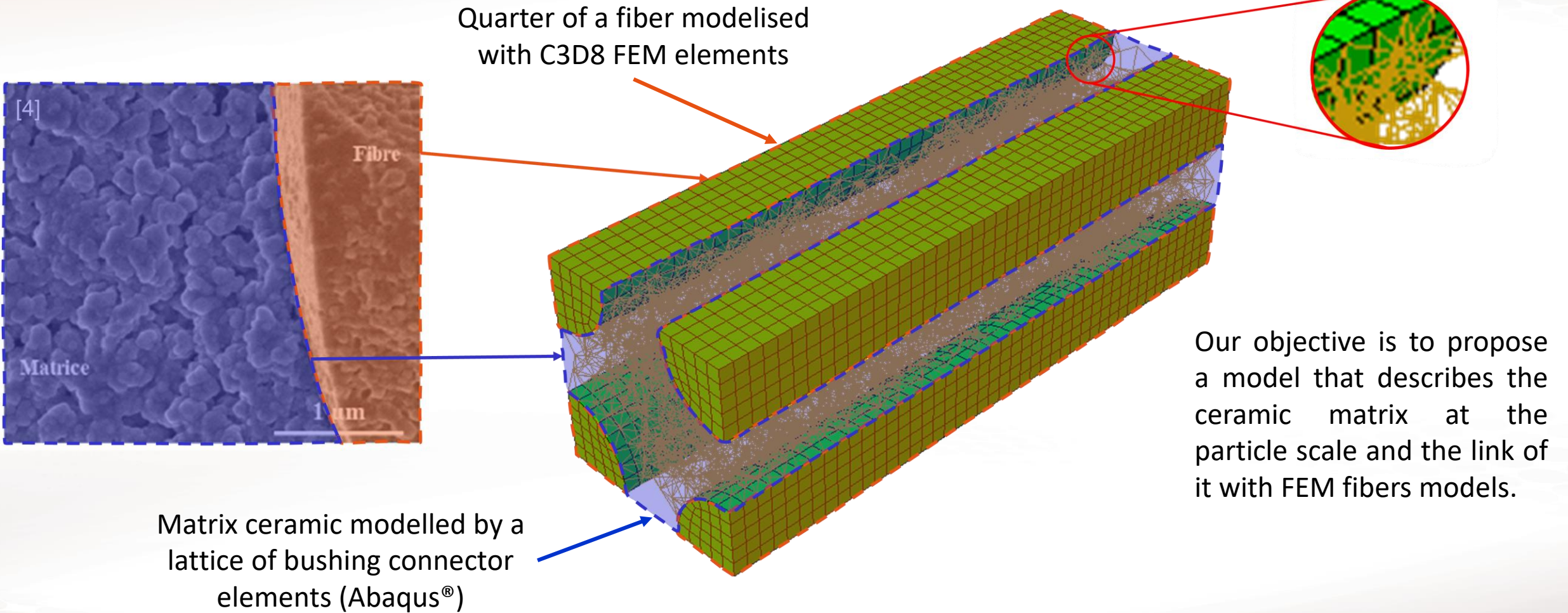
$f_{homogen} = 7295 \text{ Hz}$

Assignment of the tensile, shear, bending and torsion rigidities to each connector in function of porosity and wt.% of silica





How to model the matrix/fiber interface in order to describe the behavior of an oxide/oxide CMC at a microscopic scale?



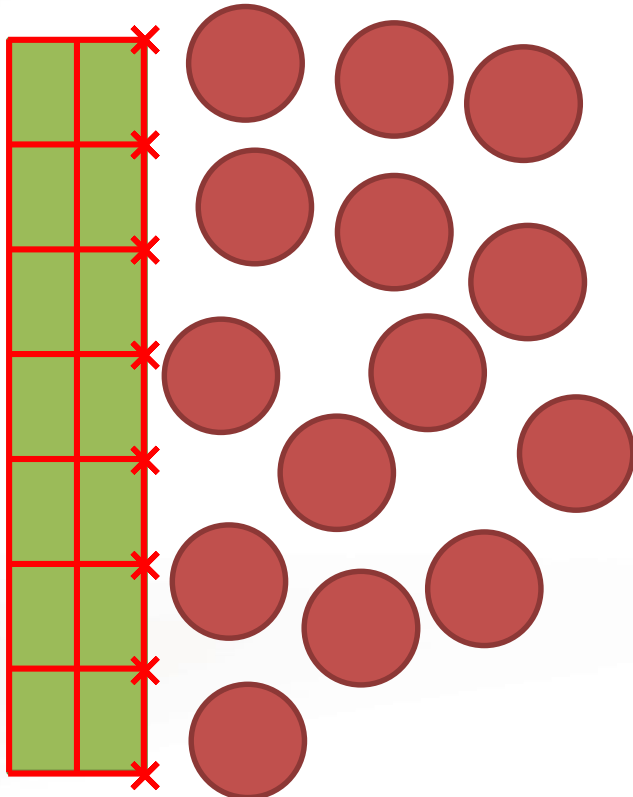
[4]: F. Boutenel, « Comportement d'une matrice alumine-silice au cours de l'élaboration de composites à matrice céramique oxyde/oxyde », novembre 202



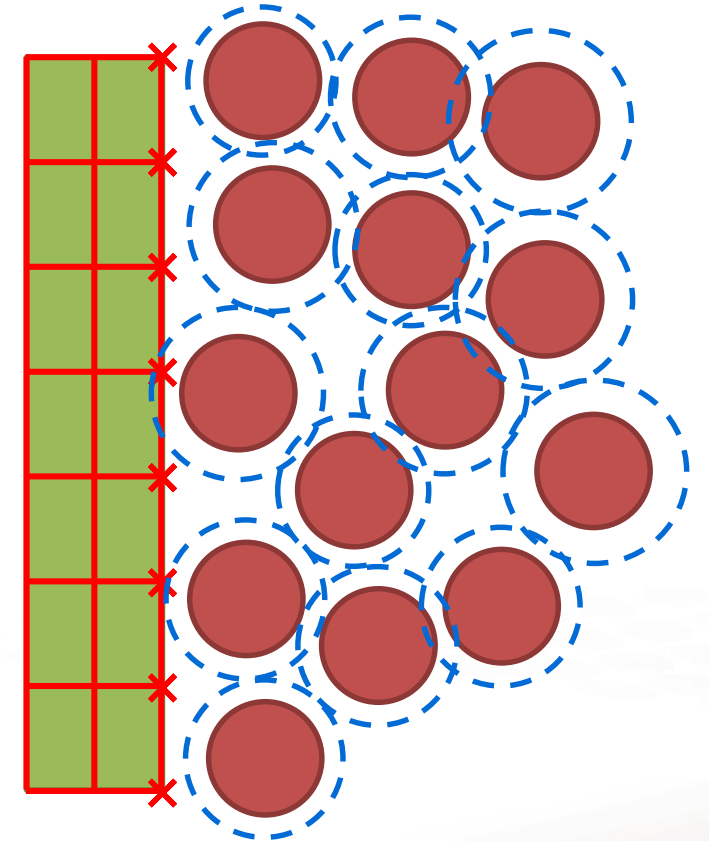
## Summary :

- Context and issues
- **Presentation of the method by lattice of connectors and FEM coupling**
  - Method of FEM/lattice connection
  - Construction of CMC Elementary Volume (EV)
- Presentation of the results
- Conclusion and outlooks






# Construction of a FEM fibres/lattice matrix link



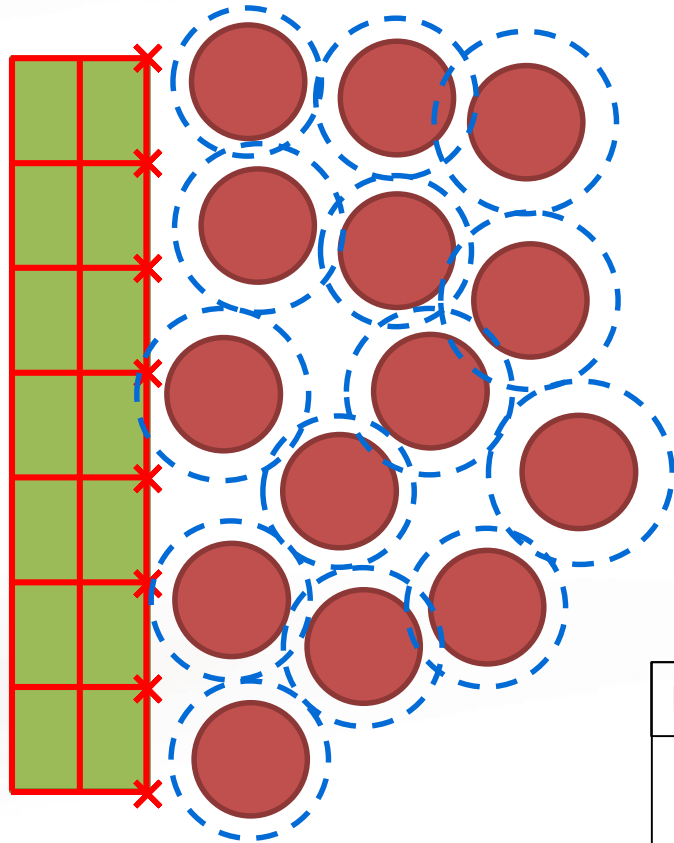
Definition of activation radii  
in function of the wt% silica



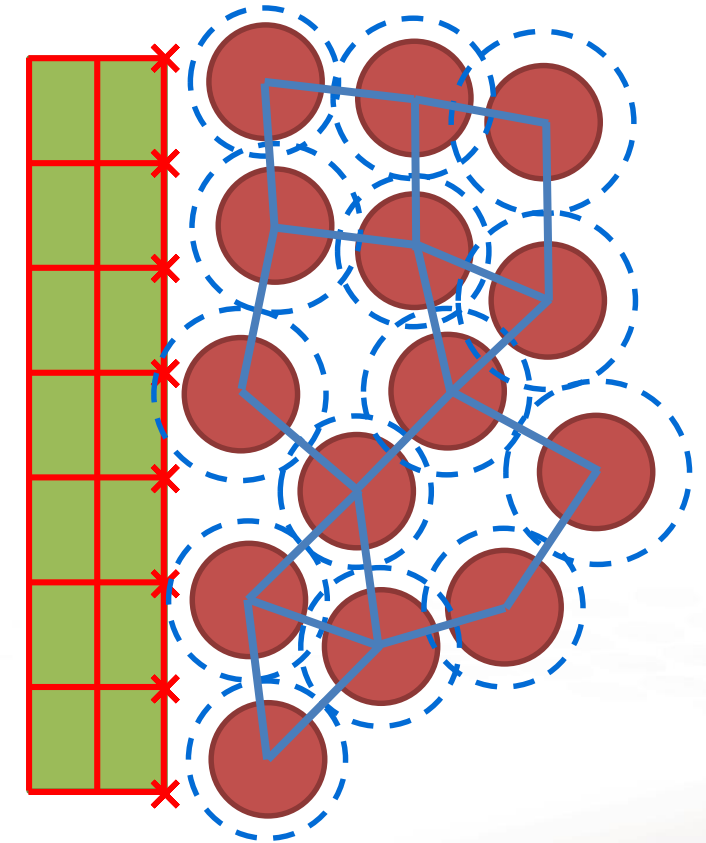
Legend :

	Alumina partilce		Alumina fiber
	FEM node		FEM element
	Particle activation radius		







# Construction of a FEM fibres/lattice matrix link



Construction of the lattice by connecting particle whom the activation radius intersect themselves

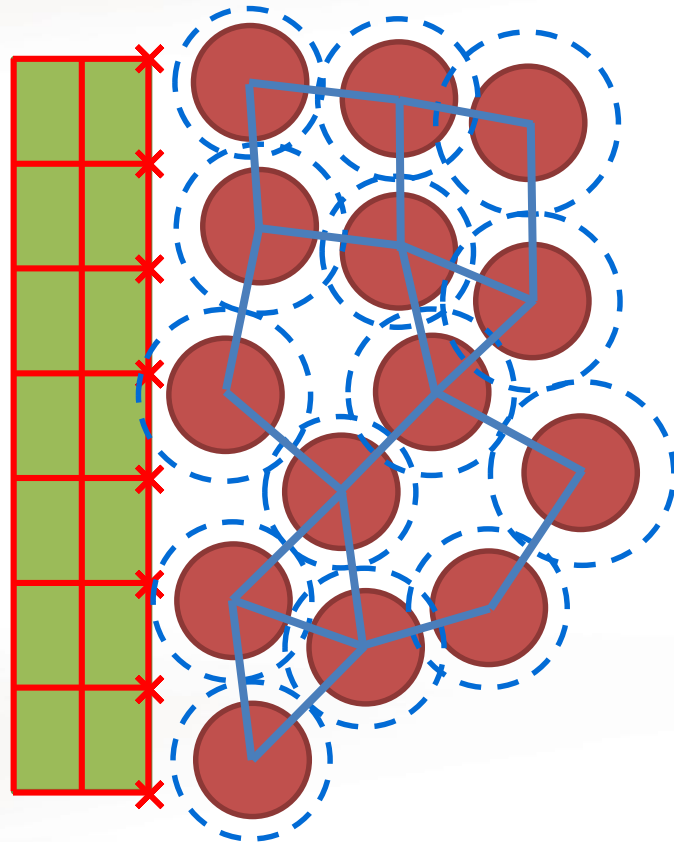


Legend :

- |   |                            |   |               |
|---|----------------------------|---|---------------|
|  | Alumina particle           |  | Alumina fiber |
|  | FEM node                   |  | FEM element   |
|  | Particle activation radius |  | Silica bridge |



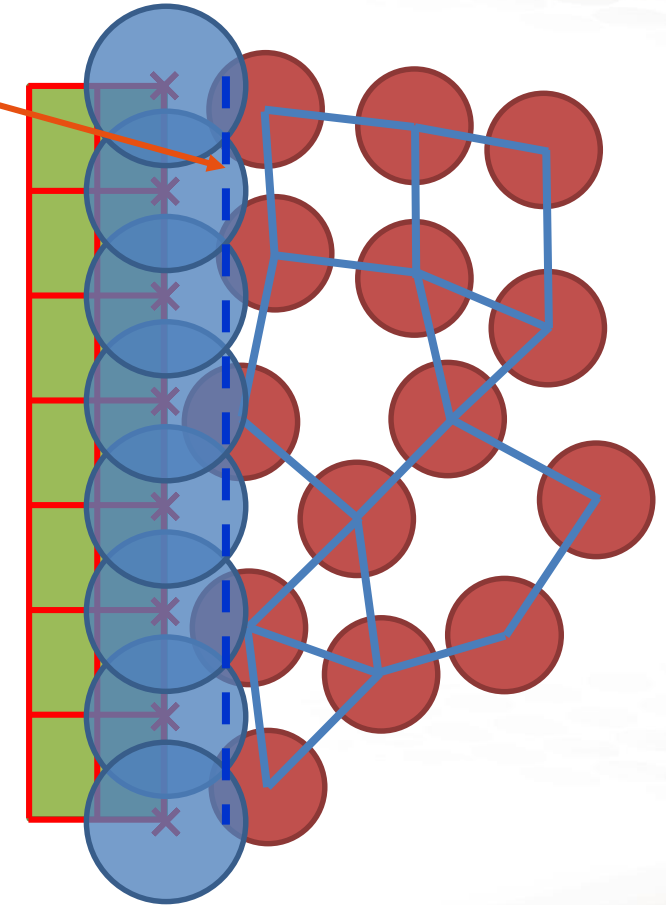
# Construction of a FEM fibres/lattice matrix link










Fiber activation zone



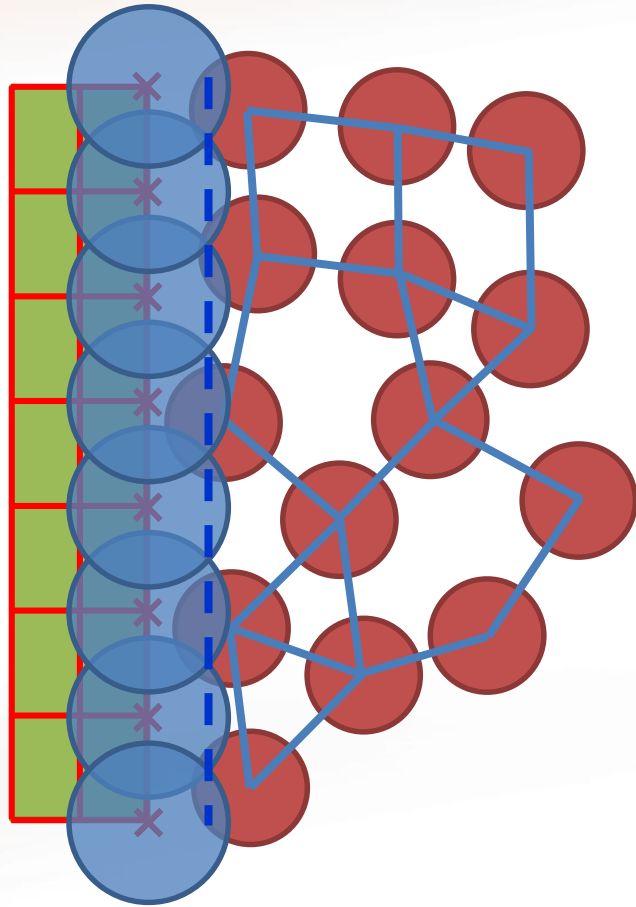
Definition of an fiber activation zone based on the particle activation radius and definition of FEM node activation radii



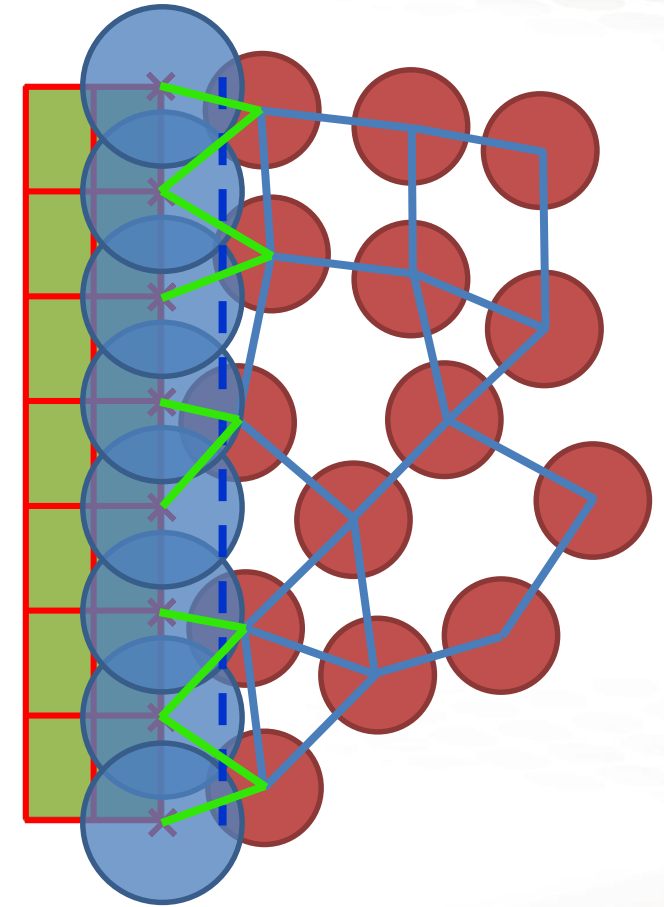
Legend :

-  Alumina particle
-  Alumina fiber
-  FEM node
-  FEM element
-  Particle activation radius
-  Silica bridge
-  FEM node activation radius









# Construction of a FEM fibres/lattice matrix link



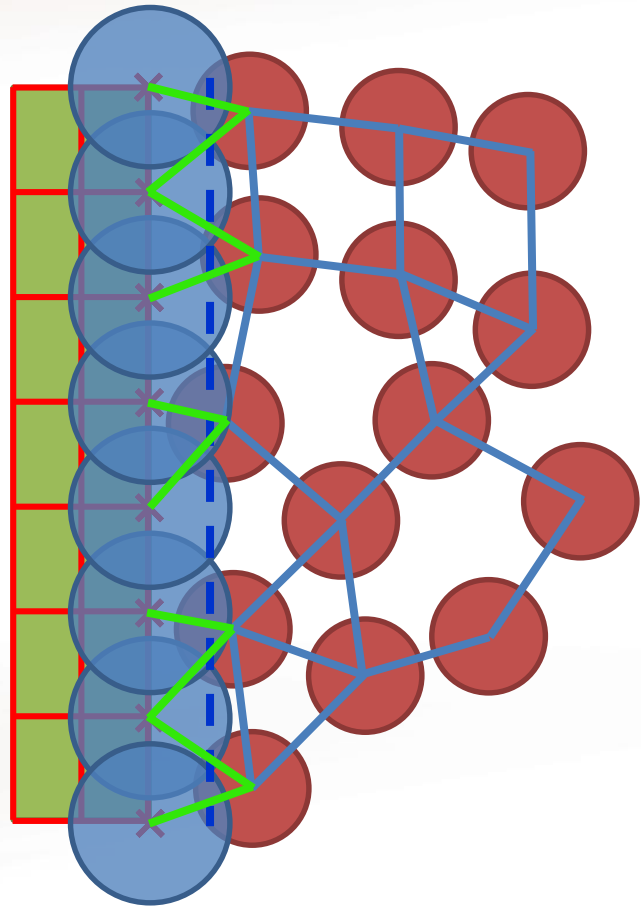
FEM node/particle connection  
if the particle is inside the FEM  
node activation radius



Legend :









 Alumina particle	 Alumina fiber
 FEM node	 FEM element
 Particle activation radius	 Silica bridge
 FEM node activation radius	 FEM fibre/lattice matrix link

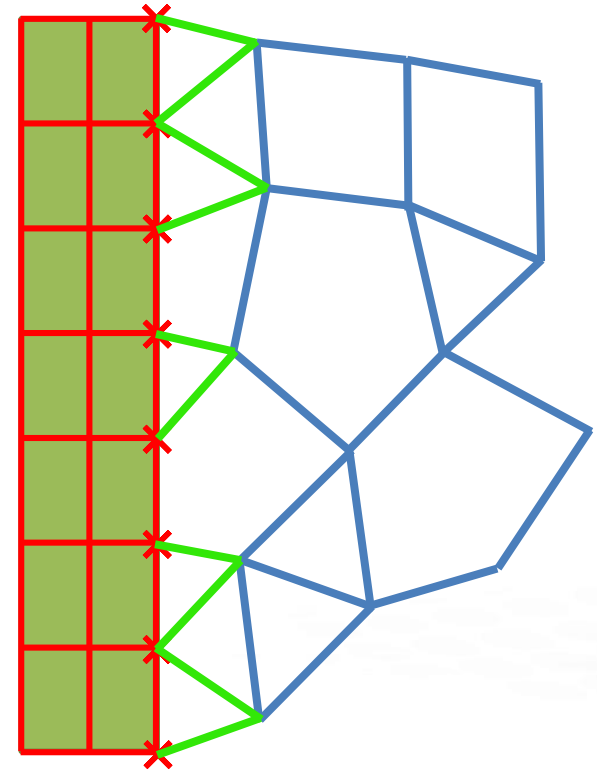
# Construction of a FEM fibres/lattice matrix link



Allocation of the rigidity to all connectors.

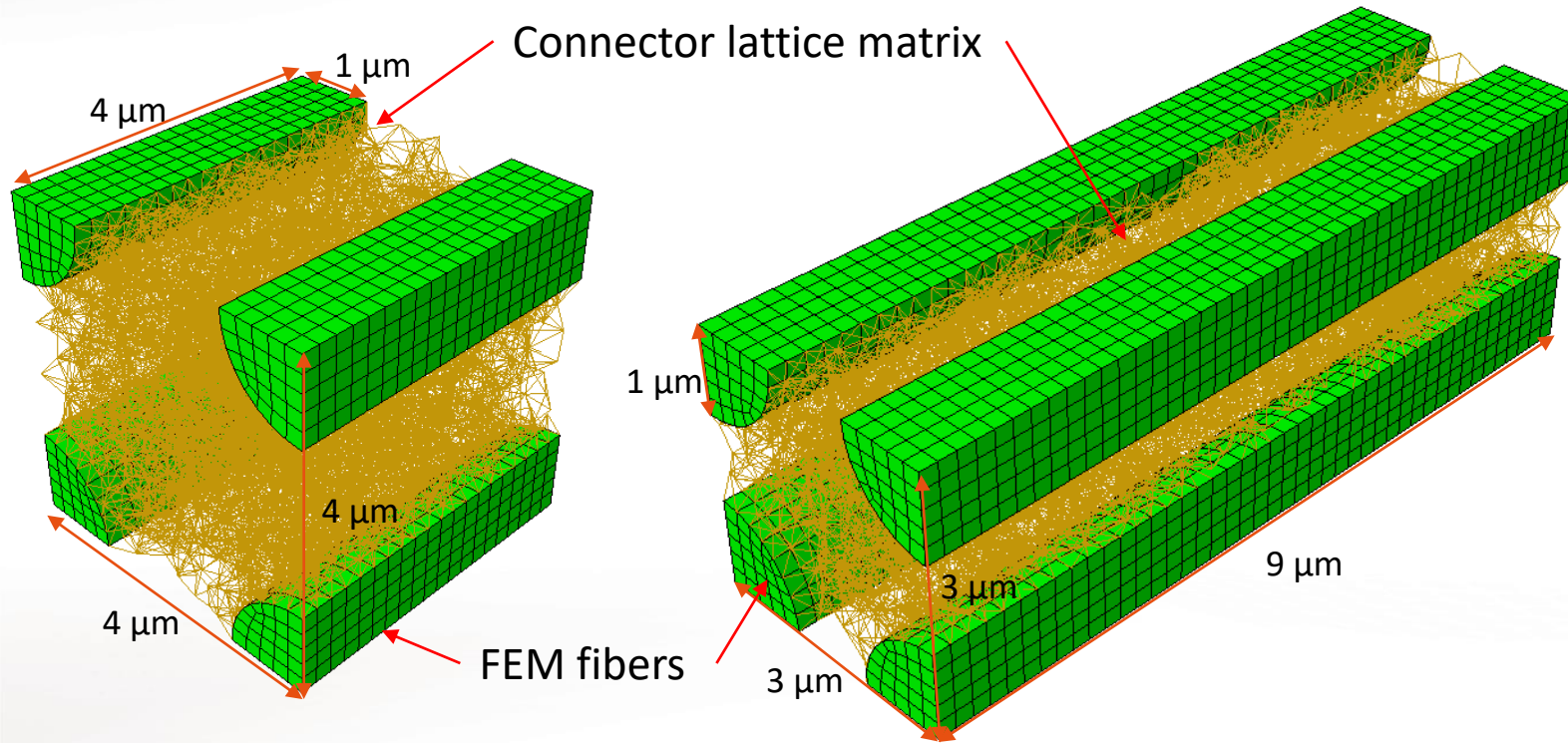
Legend :

- |  |                            |   |                               |
|--|----------------------------|---|-------------------------------|
|    | Alumina particle           |    | Alumina fiber                 |
|  | FEM node                   |  | FEM element                   |
|  | Particle activation radius |  | Silica bridge                 |
|  | FEM node activation radius |  | FEM fibre/lattice matrix link |





# Examples of a coupled FEM fiber/lattice matrix model



Microstructure which will be used in a tensile test  
%vol. fiber= 20%

Microstructure which will be used in a modal analysis  
%vol. fiber= 35%

	Hybrid tensile model	Hybrid modal analysis
Number of FEM elements (C3D8)	1920	4224
Number of lattice connectors	6559	5826
Number of lattice/FEM connectors	2819	5911
Number of FEM connected nodes	491	1043

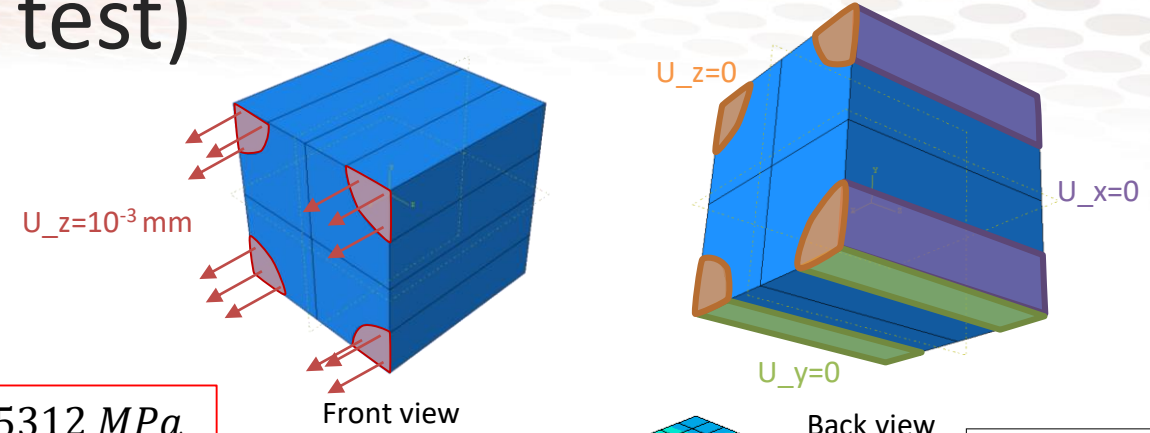
The results of these 2 analysis will be compared to an equivalent continuous model

## Summary :

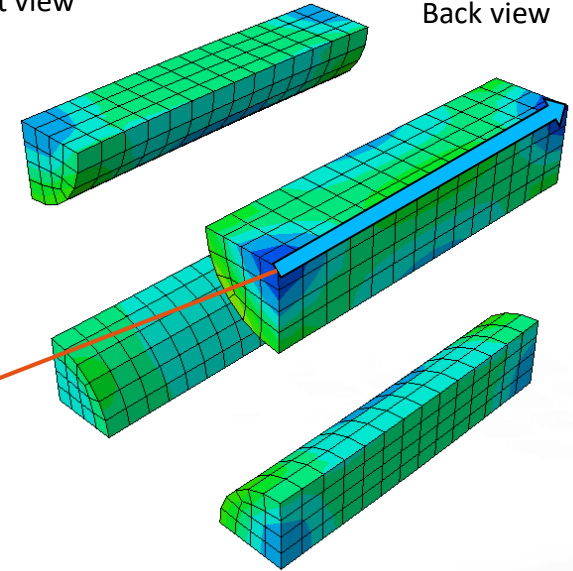
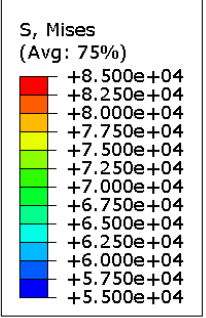
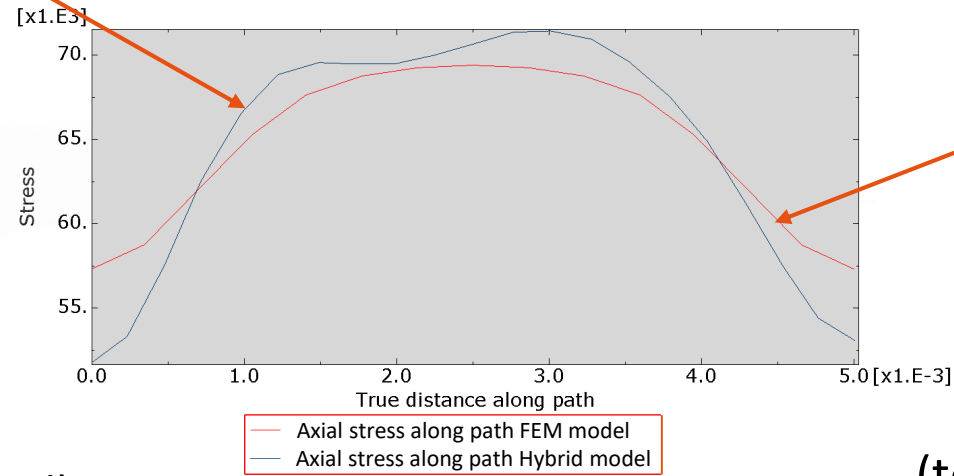
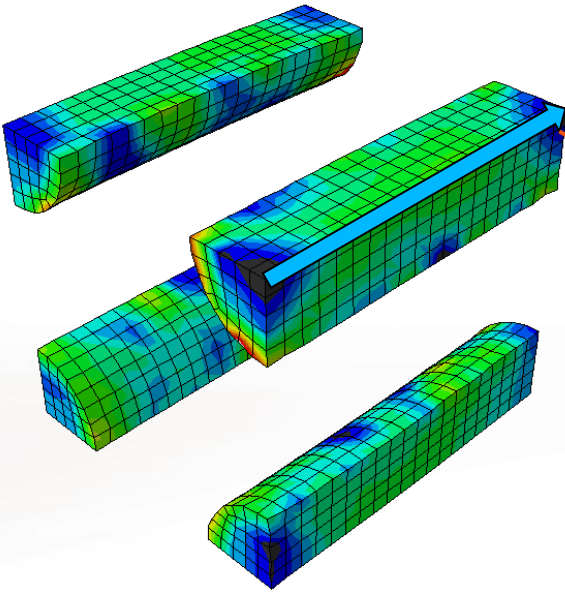
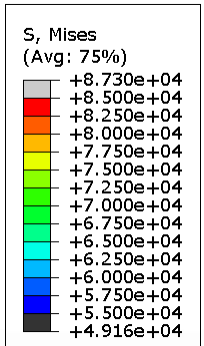
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# Results of the FEM fibers/lattice model (tensile test)

Stress fields obtained by a traction test of a 28% porous matrix with 28 wt.% silica content. The continuous matrix properties are obtained from the previous homogenization method.



$S_{33} \text{ mean hybrid} = 65312 \text{ MPa}$   
 $S_{33} \text{ mean FEM} = 65081 \text{ MPa}$   
 Relative deviation = 0,36%



Hybrid model  
(tensile test by displacement control)

Calculus time  $\approx$  30 min  
(intel core i5 1,6 GHz ; 16 Go RAM)

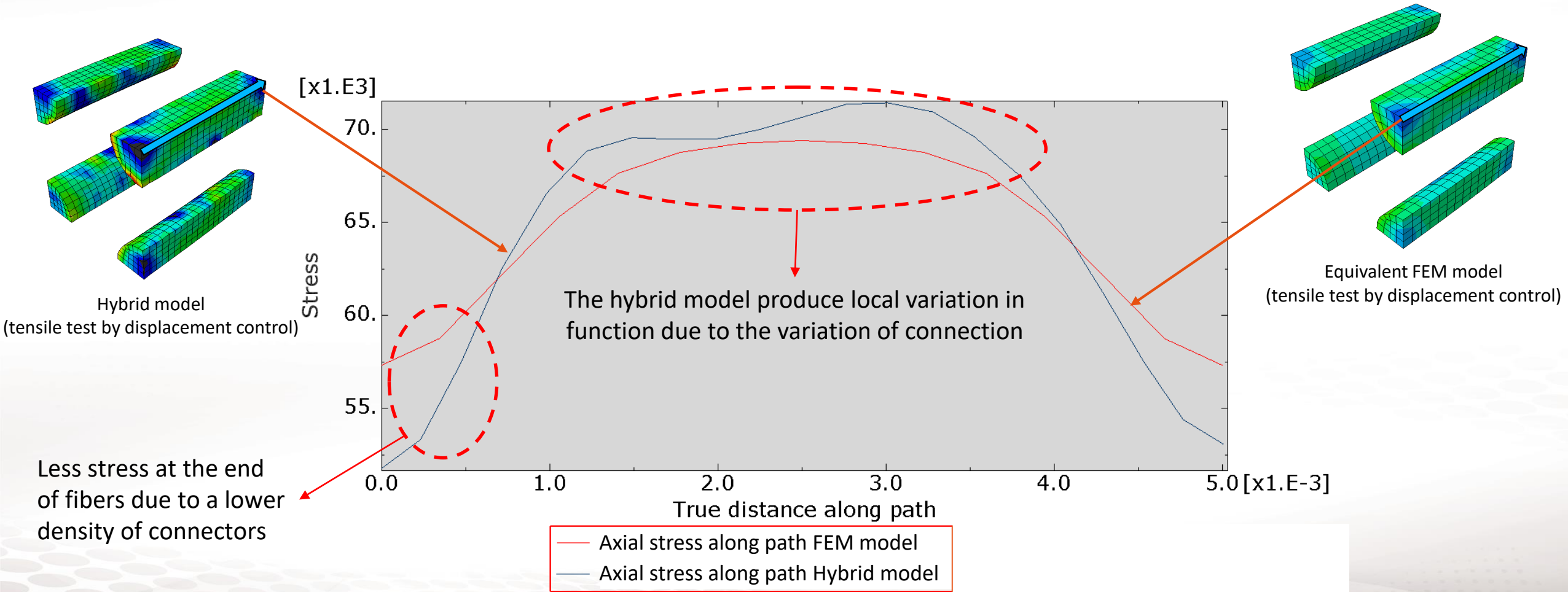
Equivalent FEM model  
(tensile test by displacement control)

Calculus time  $\approx$  30 min  
(intel core i5 1,6 GHz ; 16 Go RAM)



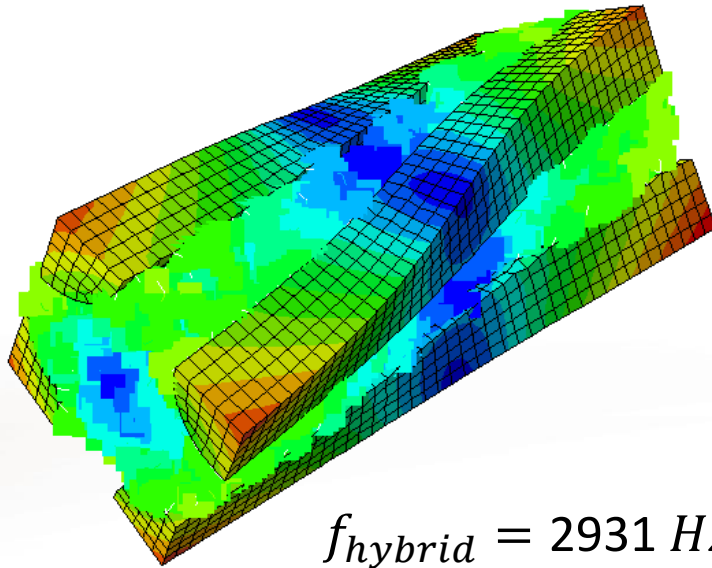
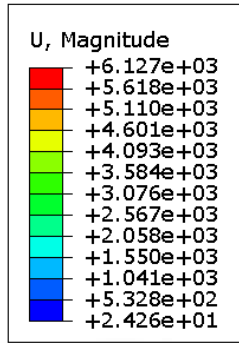
# Results of the FEM fibers/lattice model (tensile test)

Presentation and discussion of the stress distribution along the fiber for both models.



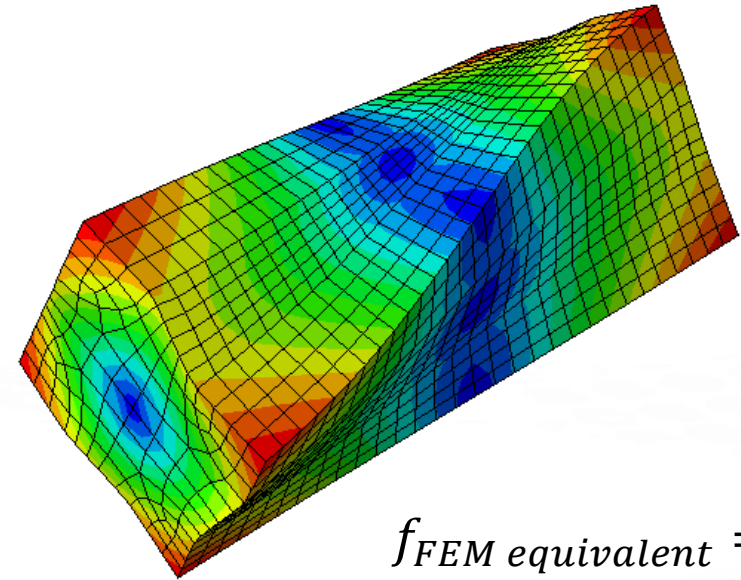
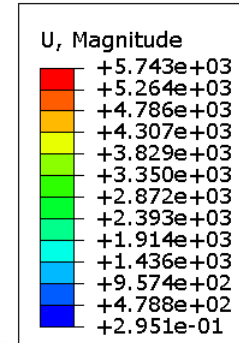
Displacement fields obtained after a modal analysis conducted on a hybrid model and a fully continuous model for a 28% porous matrix with 28 wt.% silica content.

The continuous matrix properties are obtained from the previous homogenization method.



Hybrid model (torsion eigenmode n°1)

Calculus time  $\approx$  30 min  
(intel core i5 1,6 GHz ; 16 Go RAM)

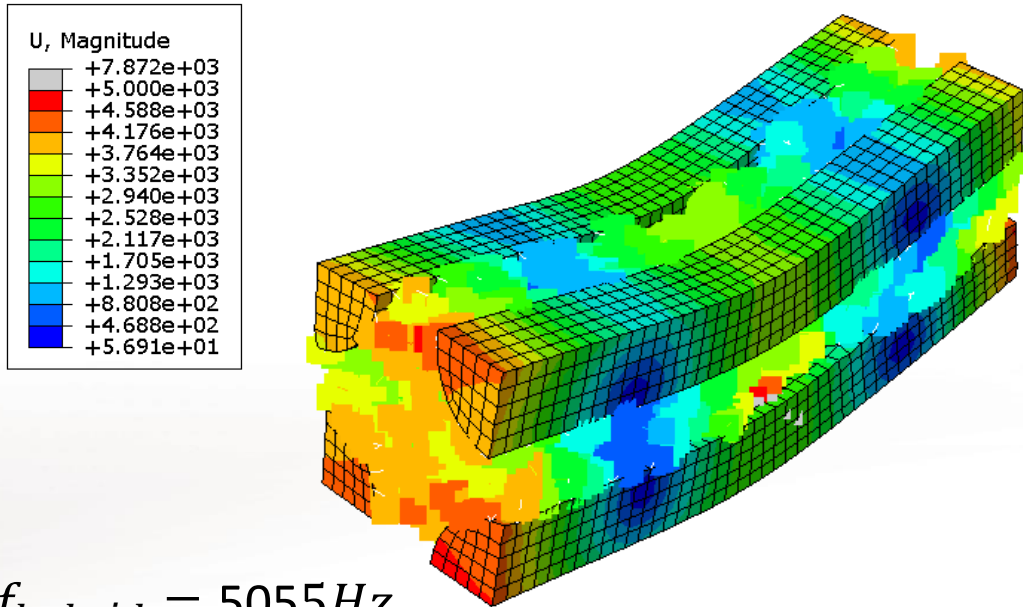


Equivalent FEM model (torsion eigenmode n°1)

Calculus time  $\approx$  40s  
(intel core i5 1,6 GHz ; 16 Go RAM)

Displacement fields obtained after a modal analysis conducted on a hybrid model and a fully continuous model for a 28% porous matrix with 28 wt.% silica content.

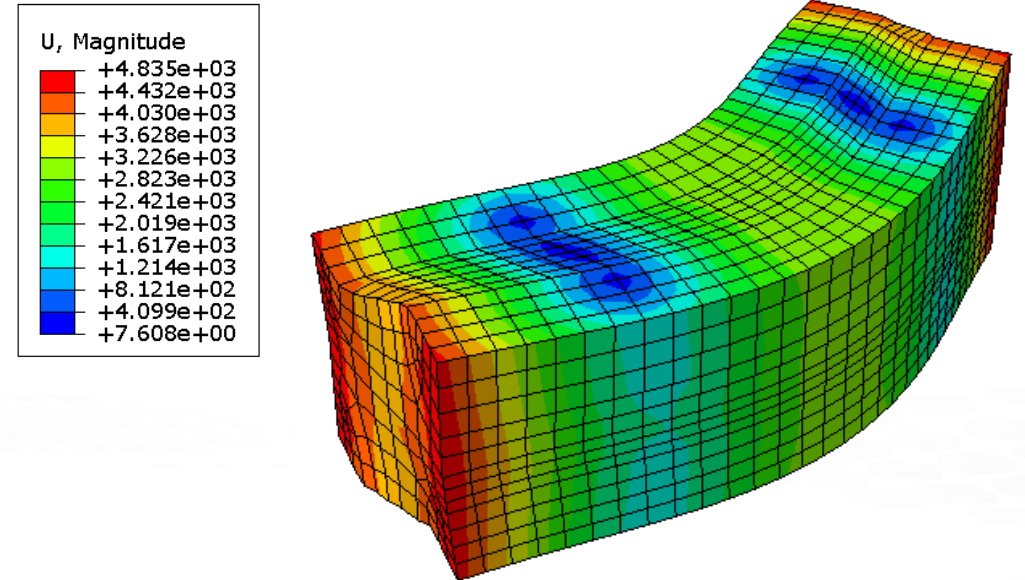
The continuous matrix properties are obtained from the previous homogenization method.



$$f_{\text{hybrid}} = 5055 \text{ Hz}$$

Hybrid model (bending eigenmode n°1)

Calculus time  $\approx$  30 min  
(intel core i5 1,6 GHz ; 16 Go RAM)



$$f_{\text{FEM equivalent}} = 5324 \text{ Hz}$$

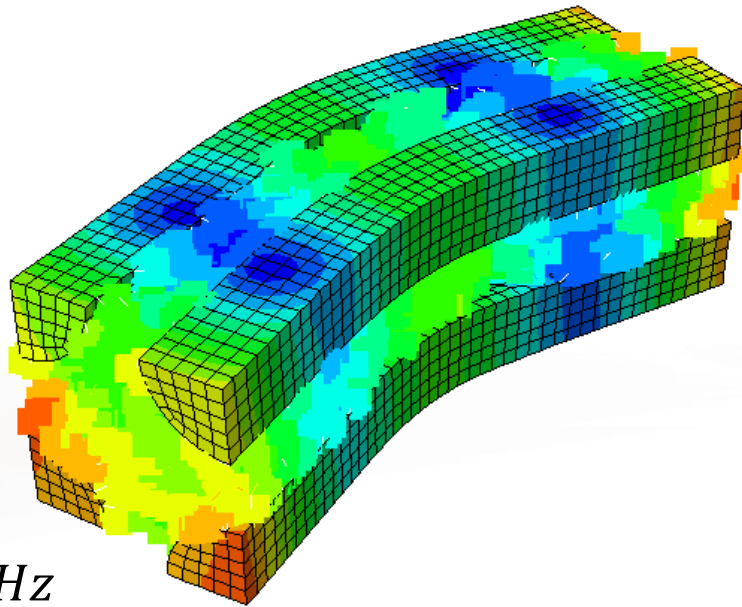
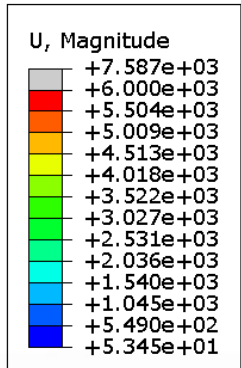
Equivalent FEM model (bending eigenmode n°1)

Calculus time  $\approx$  40s  
(intel core i5 1,6 GHz ; 16 Go RAM)



Displacement fields obtained after a modal analysis conducted on a hybrid model and a fully continuous model for a 28% porous matrix with 28 wt.% silica content.

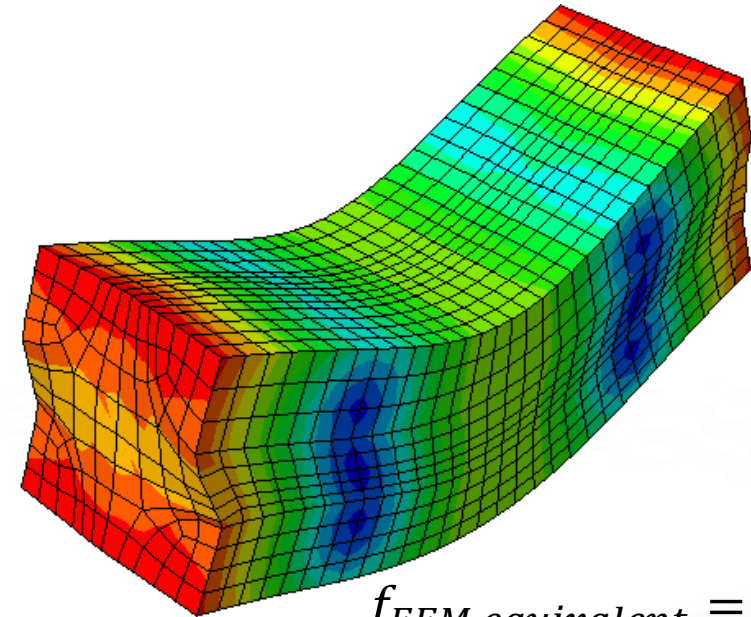
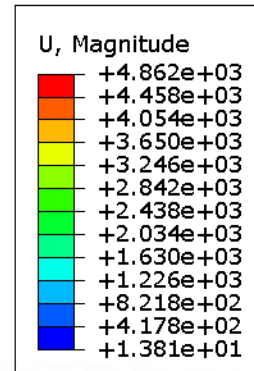
The continuous matrix properties are obtained from the previous homogenization method.



$$f_{hybrid} = 5124 \text{ Hz}$$

Hybrid model (bending eigenmode n°2)

Calculus time  $\approx$  30 min  
(intel core i5 1,6 GHz ; 16 Go RAM)



$$f_{FEM \text{ equivalent}} = 5335 \text{ Hz}$$

Equivalent FEM model (bending eigenmode n°2)

Calculus time  $\approx$  40s  
(intel core i5 1,6 GHz ; 16 Go RAM)

# Results of the FEM fibers/lattice model (modal analysis)

Comparison between the results of modal analysis of both models

	<b>Hybrid model</b> (Frequency in Hz)	<b>Equivalent FEM model</b> (Frequency in Hz)	<b>Relative deviation</b>
Torsion eigenmode n°1	2931,3	3334,1	13,7%
Bending eigenmode n°1	5054,9	5323,7	5,3%
Bending eigenmode n°2	5124,1	5335,0	4,1%

Greater difference on torsion behavior than on bending one

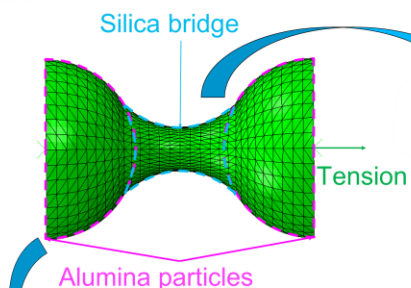
Presence of a noticeable anisotropy

## Summary :

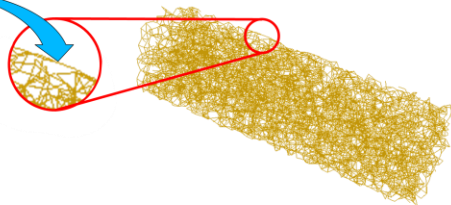
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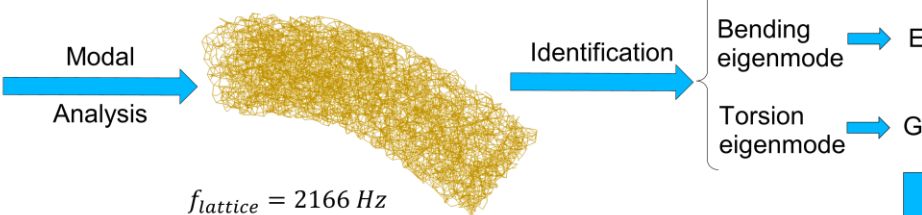
**a. Mechanical modelling of silica bridges.**



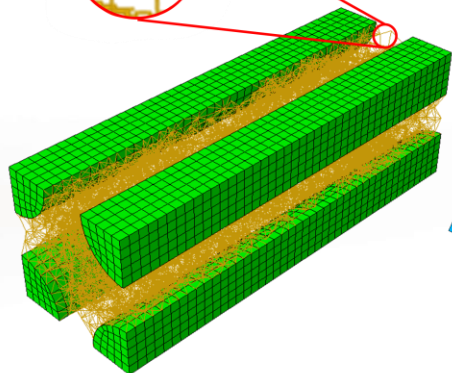
**b. Formation of a lattice connector REV and injection of silica bridges mechanical properties.**



**c. Homogenisation of the REV by modal analysis and calcul of mesoscopic mechanical properties.**

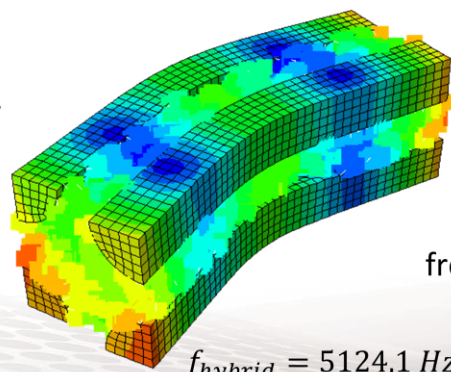


Injection of silica bridge rigidity in connectors



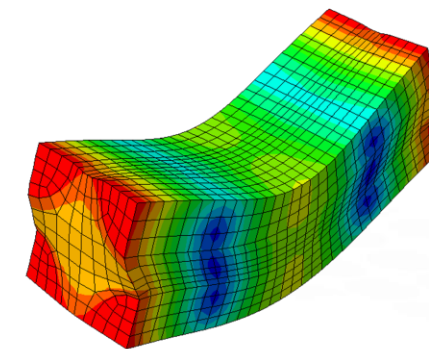
**d.1. Building of an hybrid CMC model.**

Modal Analysis



**e. Comparison of frequencies obtained with hybrid et FEM models.**

Comparison  
Frequency relative deviation ≈ 4,1%



**d.2. Building of a FEM equivalent CMC model.**

$f_{FEM \text{ equivalent}} = 5335 \text{ Hz}$

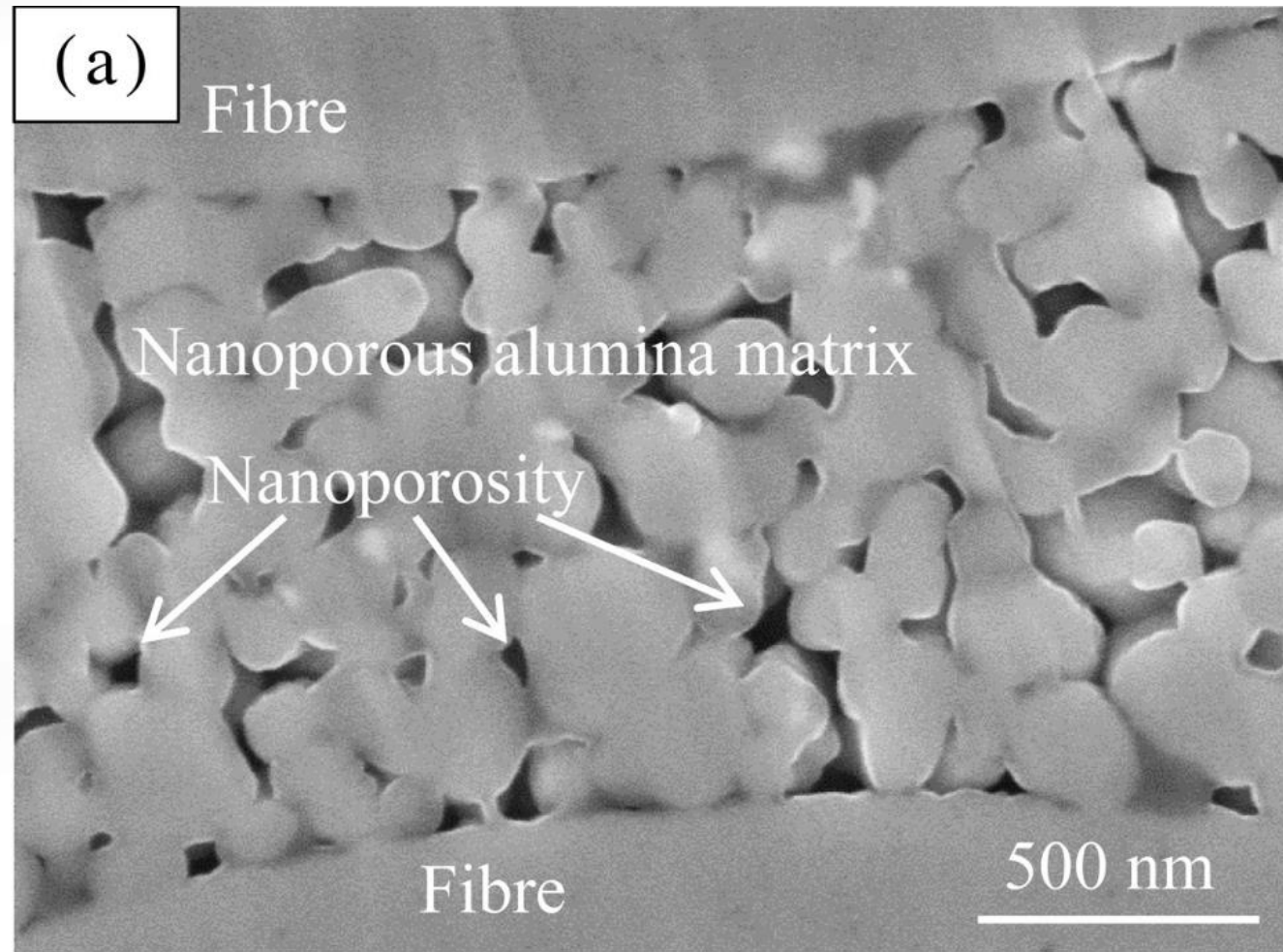
- Improving the numerical method
  - Improving the lattice/FEM connection method and give to it a physical meaning
- Comparison with experiments
  - For the homogenisation method applied to the matrix alone (in progress)
  - For the CMC hybrid method.
- Development of the method :
  - Enhancement of connector behaviour (viscoplasticity, sintering)

# Thanks for your attention

Acknowledgements: This research received a grant from the Occitanie region and fundings from IMT Mines Albi.







According to the article of Osvald André Quaglio et al. the Young modulus can be deduced of the bending eigenmodes of a cylindrical beam through the following formula :

$$E = 1,6067 \left( \frac{L^3}{D^4} \right) (m f_f^2) T_1'$$

$$T_1' = 1 + 4,939(1 + 0,0752\nu + 0,8109\nu^2) \left( \frac{D}{L} \right)^2 - 0,4883 \left( \frac{D}{L} \right)^4 - \left[ \frac{4,6911(1 + 0,2023\nu + 2,173\nu^2) \left( \frac{D}{L} \right)^4}{1,000 + 4,7541(1 + 0,1408\nu + 1,536\nu^2) \left( \frac{D}{L} \right)^2} \right]$$

Knowing that if  $\frac{L}{D} > 20$  then  $T_1' = 1,000 + 4,939 \left( \frac{D}{L} \right)^2$

Else, the Poisson coefficient can be iteratively determined with the shear modulus calculated with the torsion eigenmode through the following formula:

$$G = 4\rho L_{eff}^2 (f_{tor})^2$$

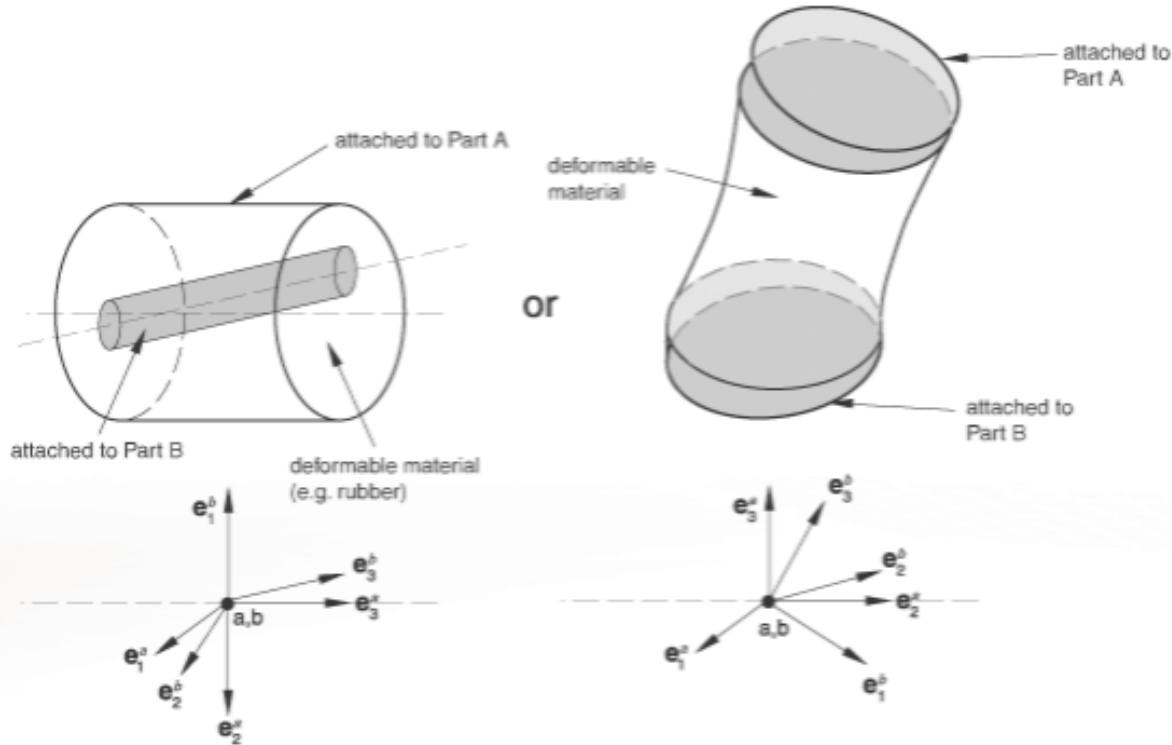
Then :

$$\nu = \frac{E}{2G} - 1$$

Quaglio et al. Determination of Young's modulus by specific vibration of basalt and diabase, *Advances in Materials Science and Engineering*, 14 avril 2020

## Description

Figure 1. Connection type BUSHING.



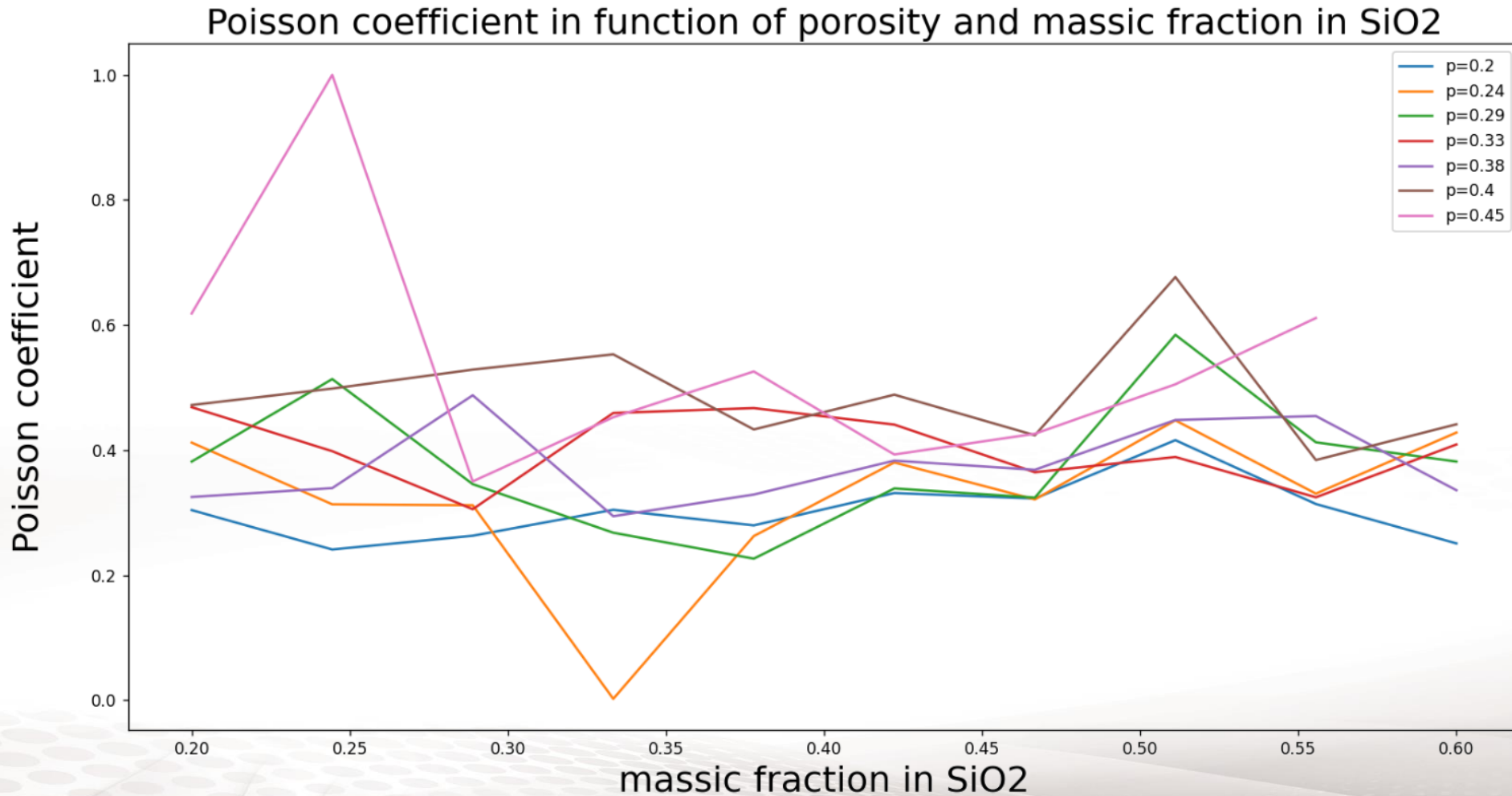
The connectors are 2-node elements in the abaqus software. The bushing type allows control of the 6 degrees of freedom of the element

[5] : Documentation Abaqus version 6,6 (section 25,1,5 connection-type library).



# Results of the homogenisation Poisson coefficient

Poisson coefficient obtained through modal homogenisation method on a connector lattice matrix for different porosities and compositions



$$\alpha = \sqrt[3]{\frac{V_{Al_2O_3}}{V_{ini}} \left(1 + \frac{v_s}{1 - v_s}\right) \left(1 + \frac{p}{1 - p}\right)}$$

Avec

$p$  : porosity

$v_s$  : Volumic fraction of silica

$V_{Al_2O_3}$  : Alumina volume in the REV

$V_{ini}$  : Volume of the REV before the homothety.

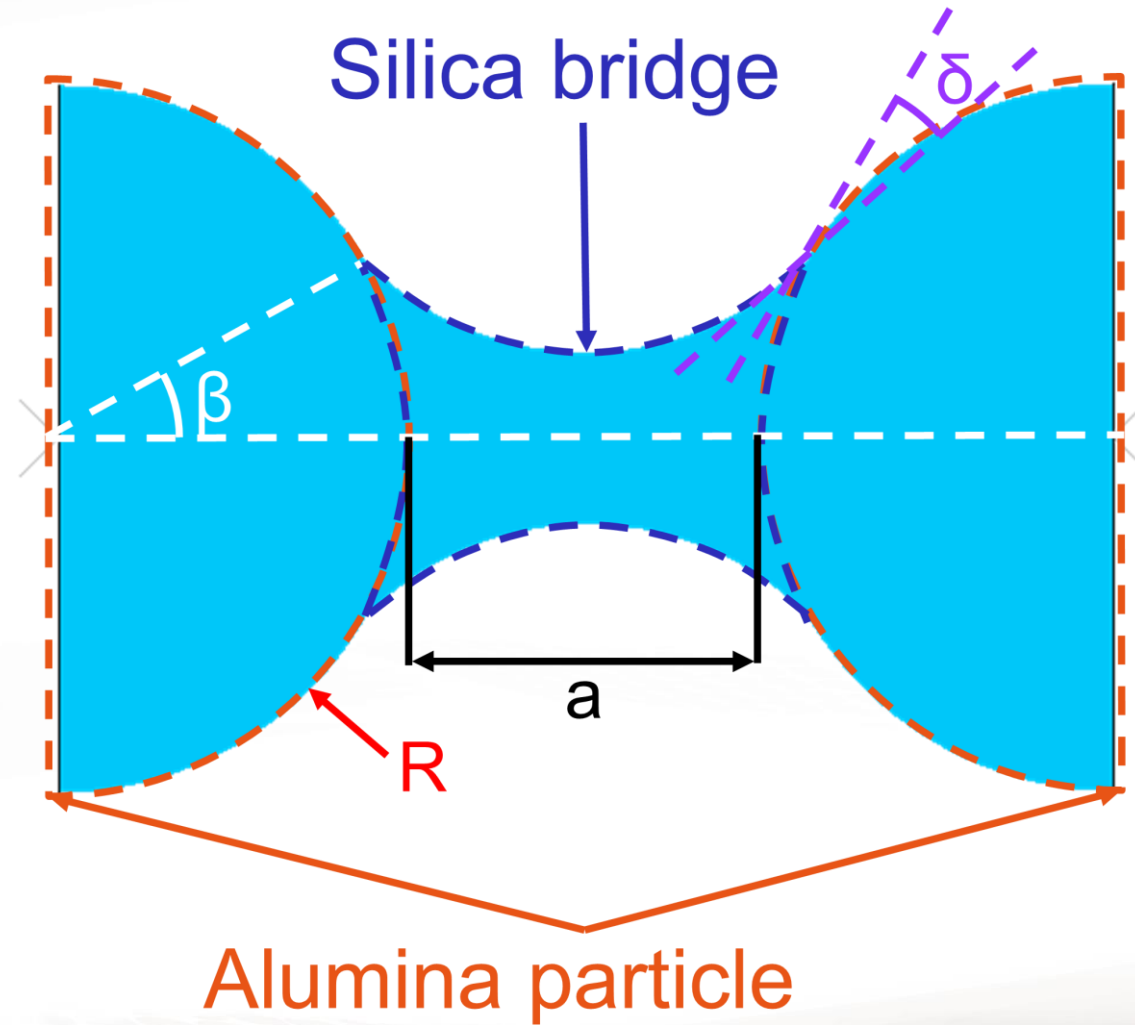
# Characteristic of the cimputer used for the numerical calculs

DELL laptop:

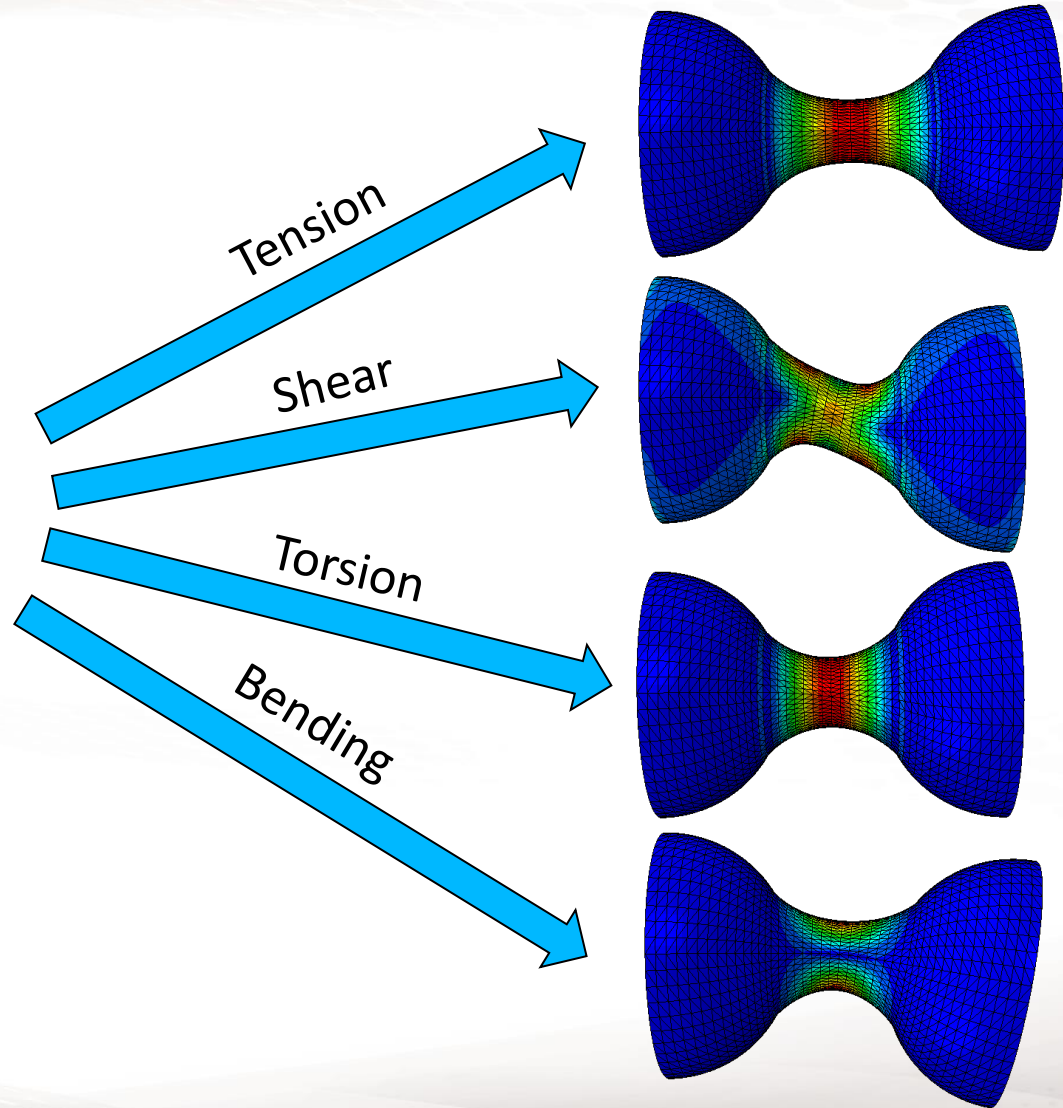
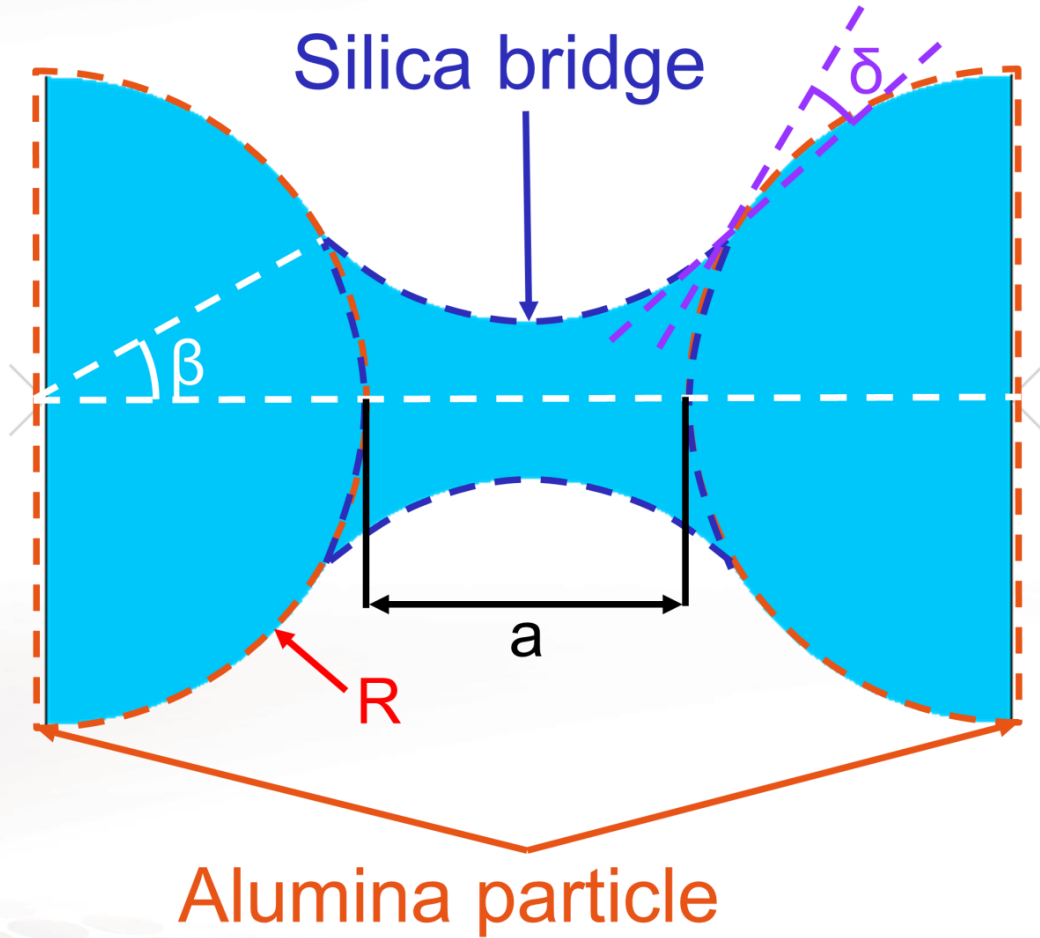
Processor : Intel(R) Core(TM) i5-10210U CPU @ 1.60GHz 2.11 GHz

RAM memory : 16,0 Go (15,6 Go utilisable)

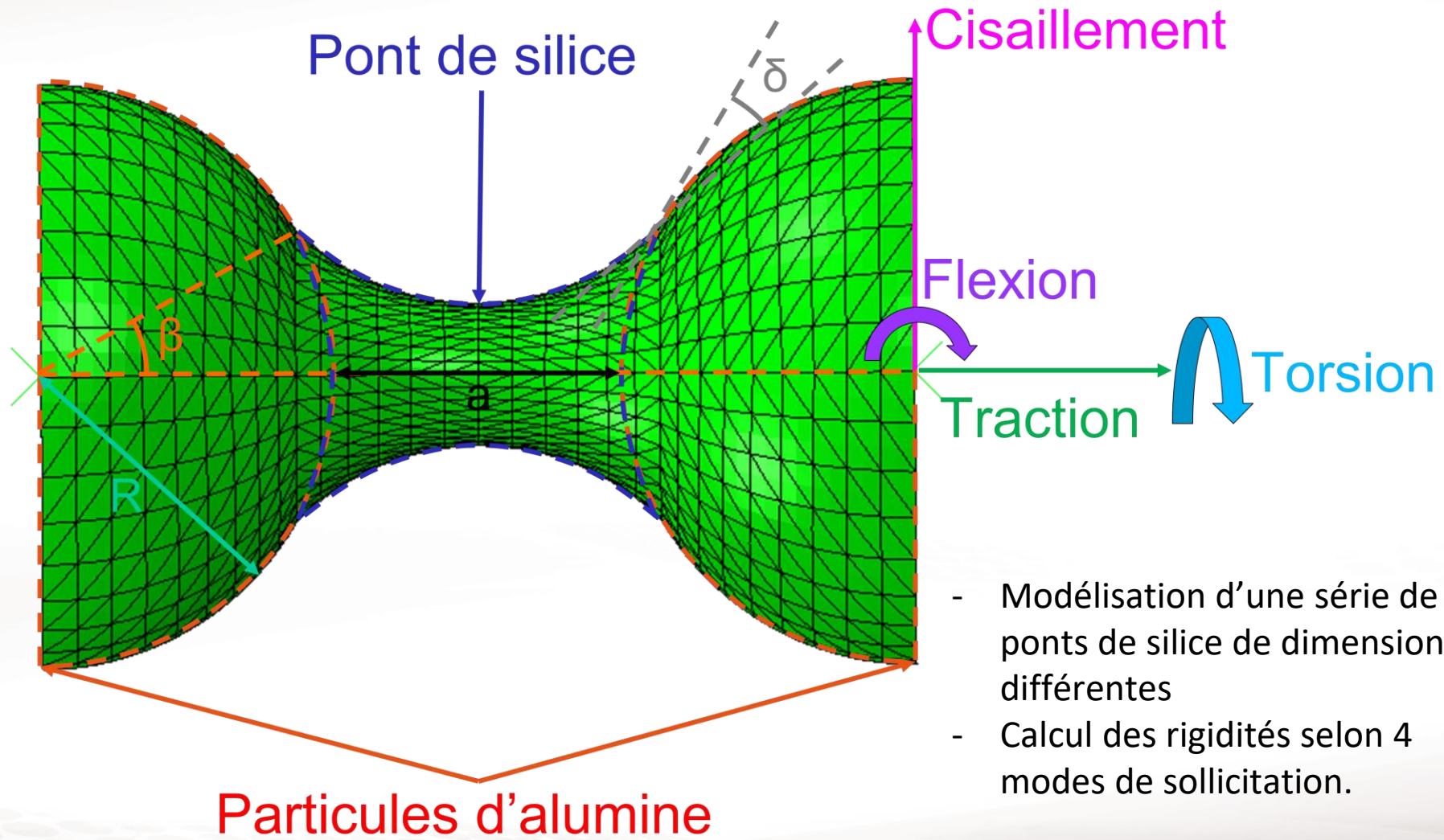




[5]: Guōping Lian et al., Journal of colloid and interface science, 11 juin 1993

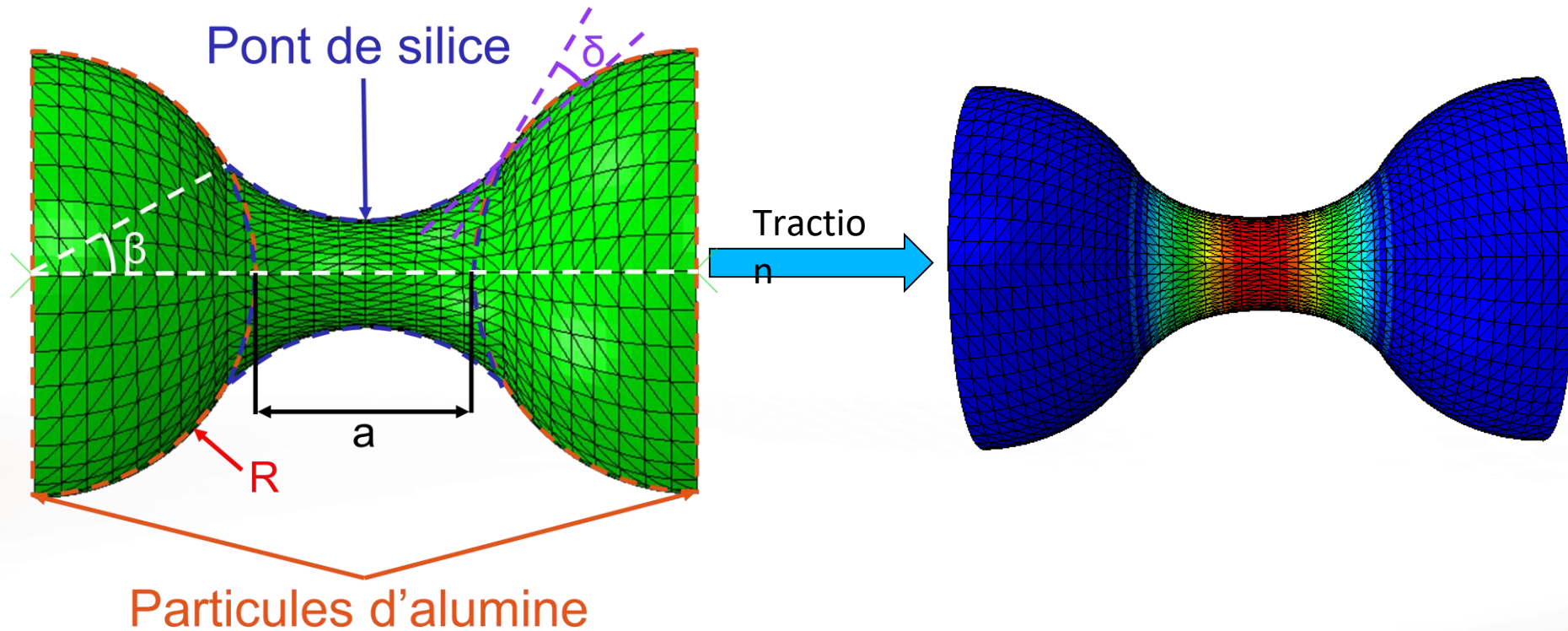


[5]: Guôping Lian et al. , Journal of colloid and interface science, 11 juin 1993

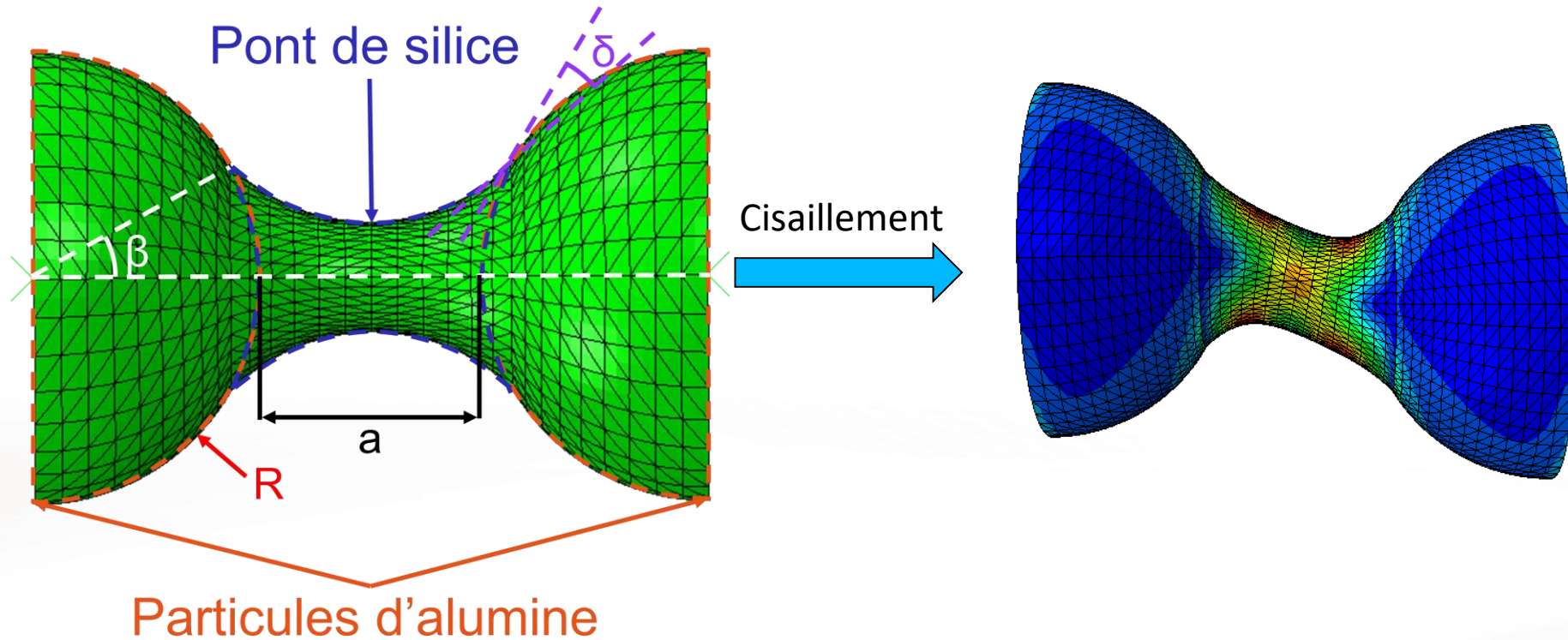


[5]: Guòping Lian et al. , Journal of colloid and interface science, 11 juin 1993



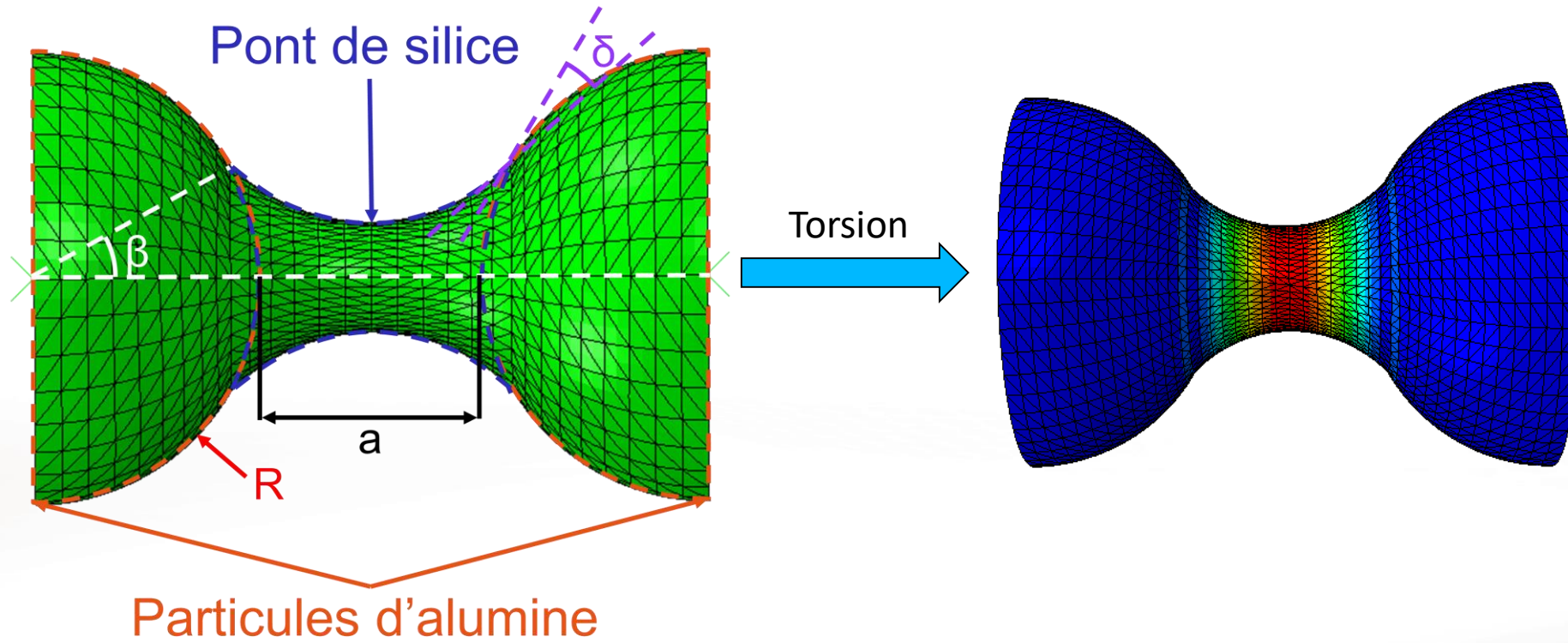


[5]: Guòping Lian et al. , Journal of colloid and interface science, 11 juin 1993



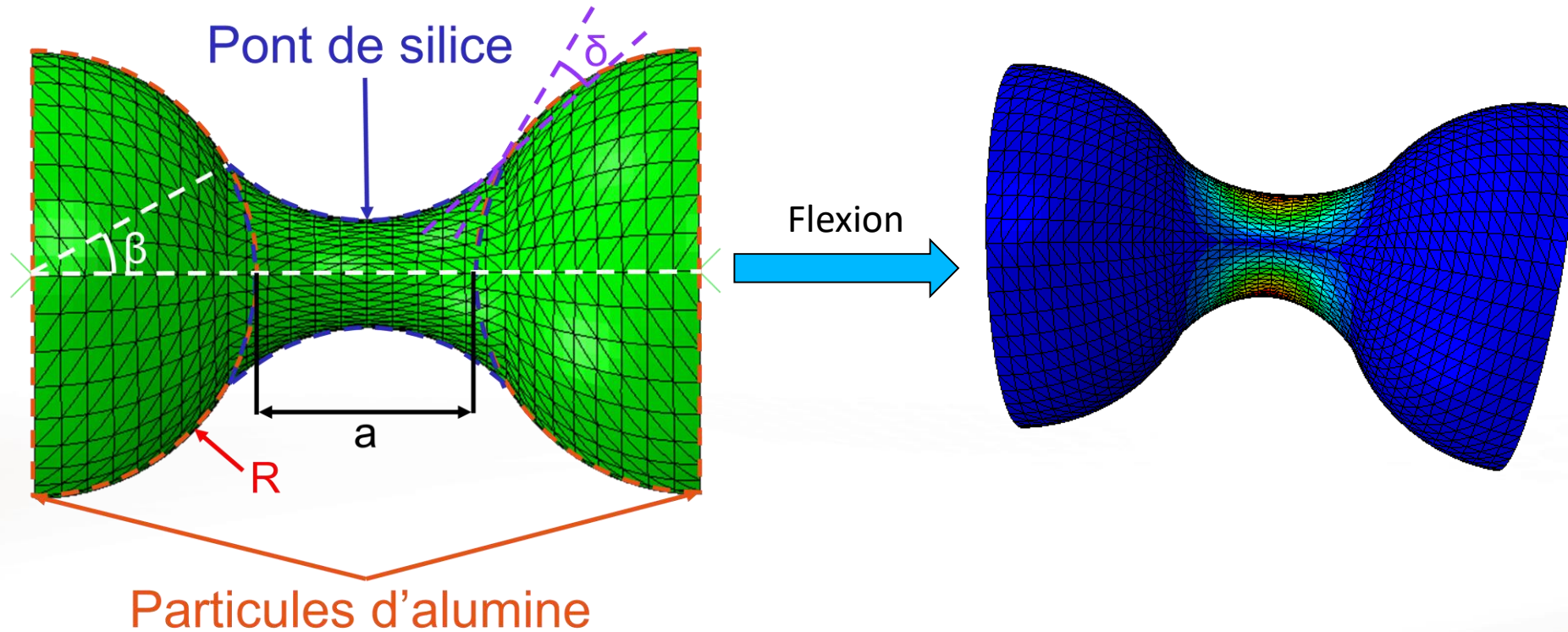
[5]: Guòping Lian et al. , Journal of colloid and interface science, 11 juin 1993





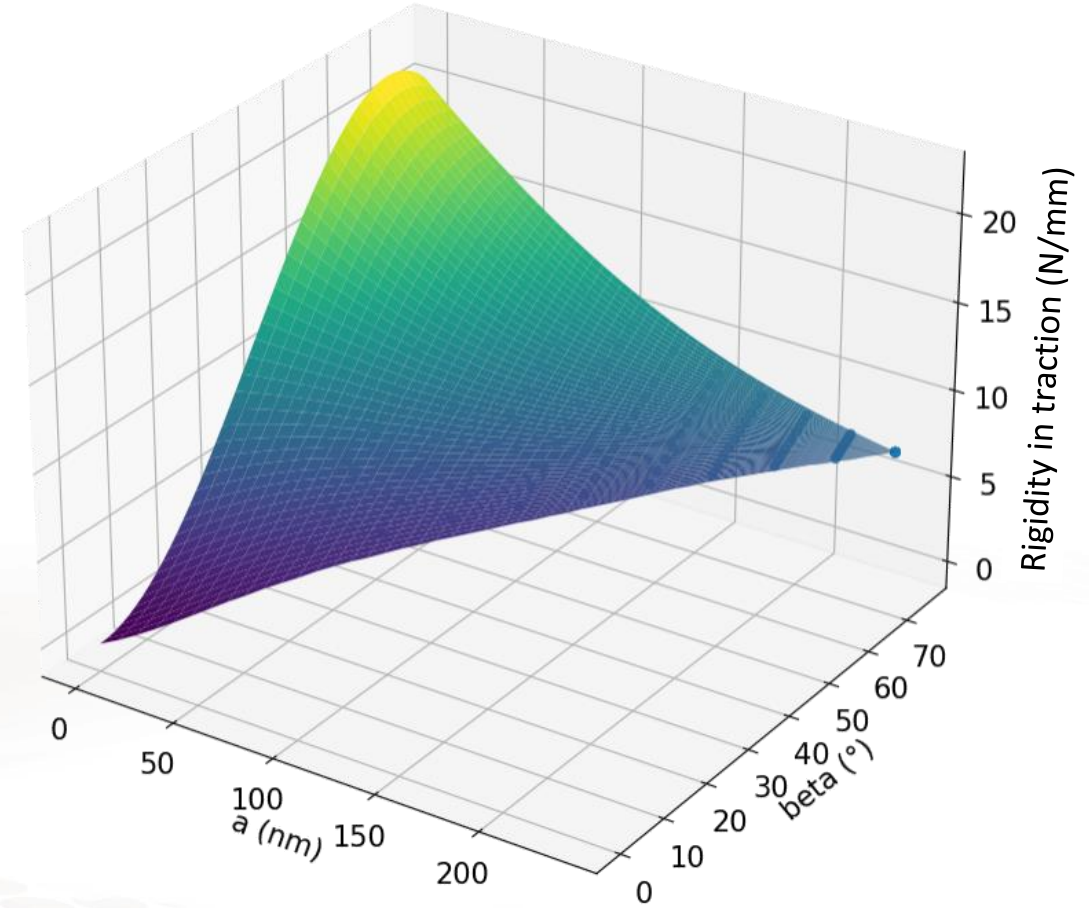
[5]: Guòping Lian et al. , Journal of colloid and interface science, 11 juin 1993





[5]: Guòping Lian et al. , Journal of colloid and interface science, 11 juin 1993

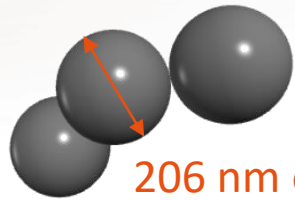
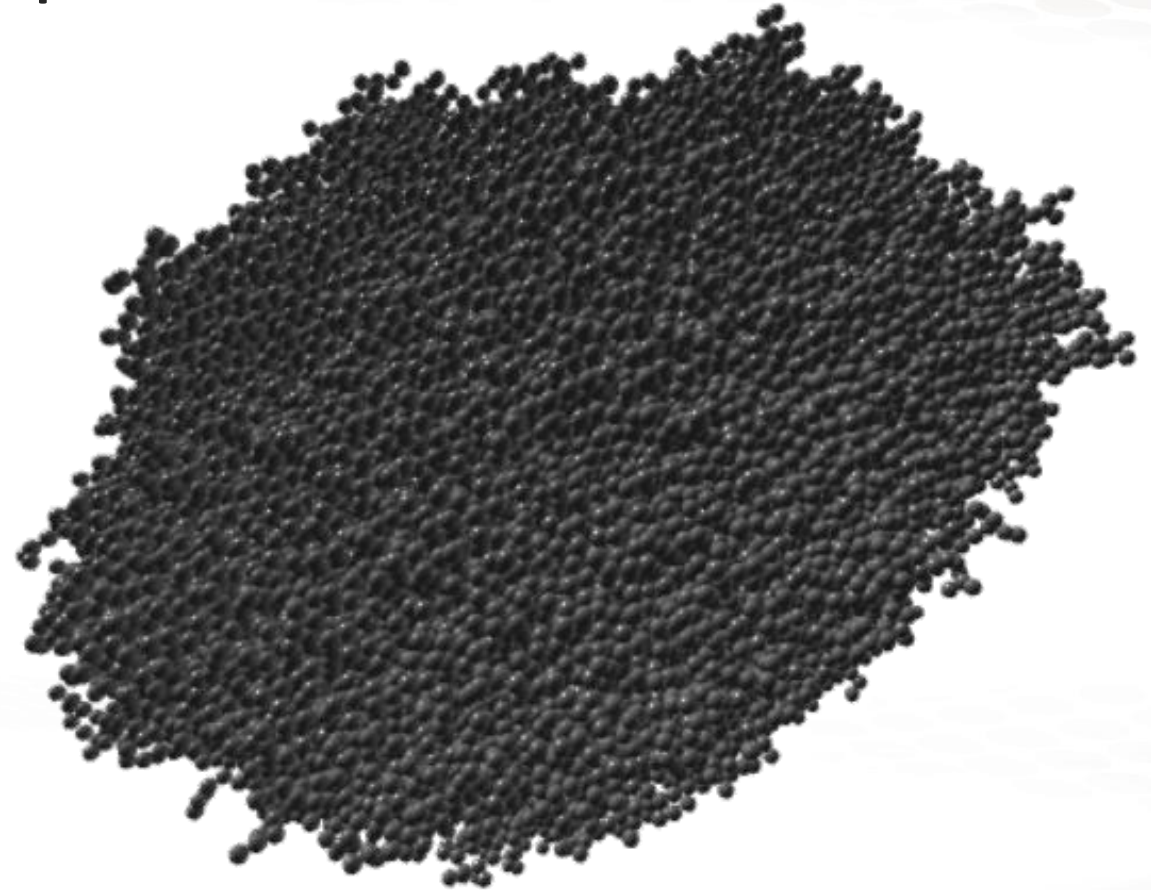
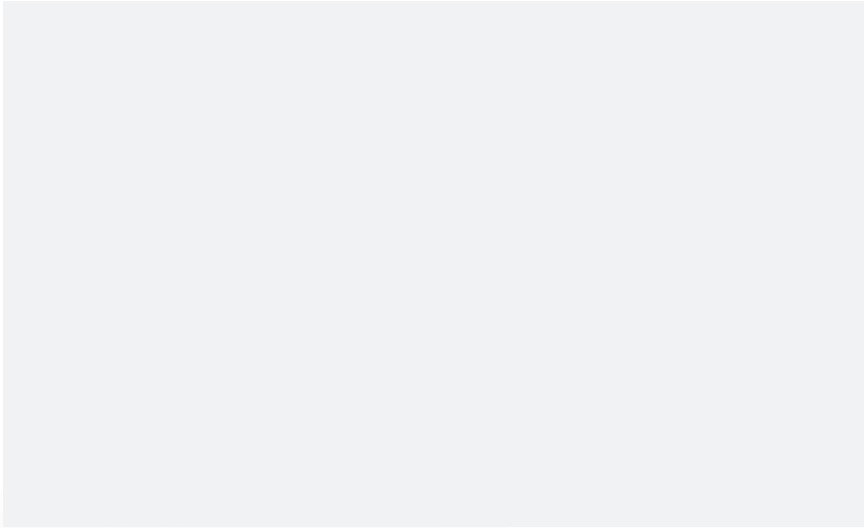
Bezier surface on rigidity (traction)



Construction of a surface response with 100 different silica bridges. (obtained by modification of  $a$  and  $\beta$ ).

The rigidity results are then fitted by an order 4 Bézier surface in both direction.

# Construction of a REV Formation of a particle cluster



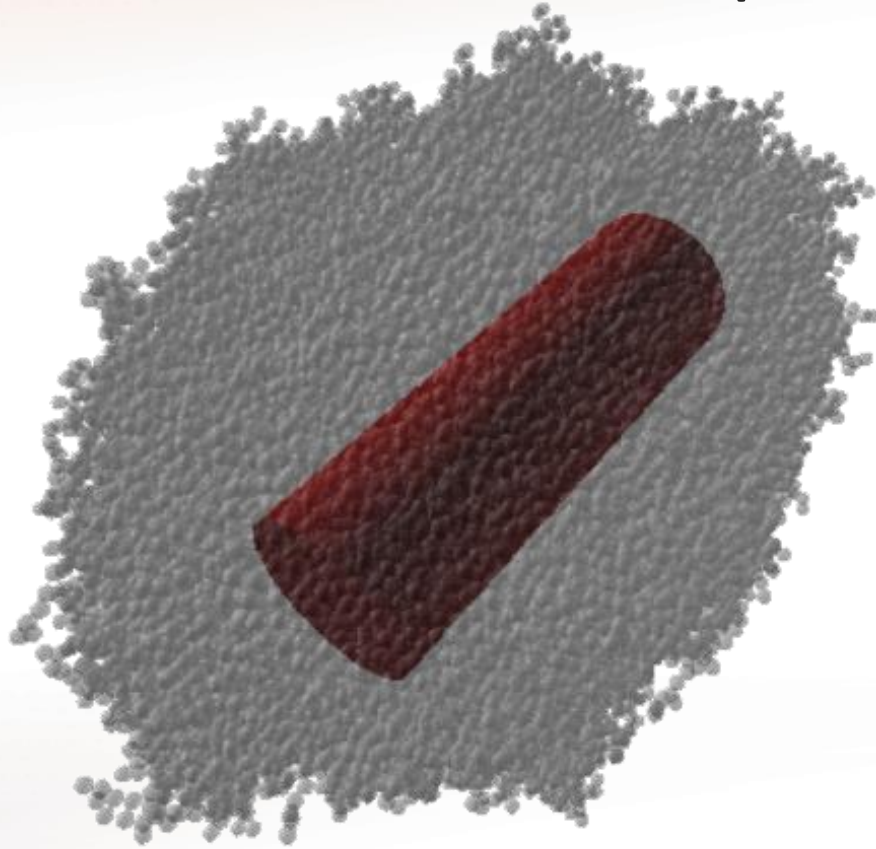
206 nm on average

Programming of an algorithm of random positioning of alumina particle in contact with each other.  
(Example of a 50000 particle cluster )

[5]: Simone Falco et al. International Journal For Numerical Methods in Engineering, 22 février 2017



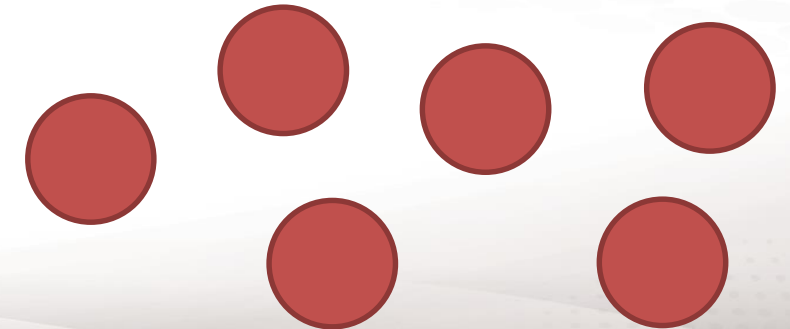
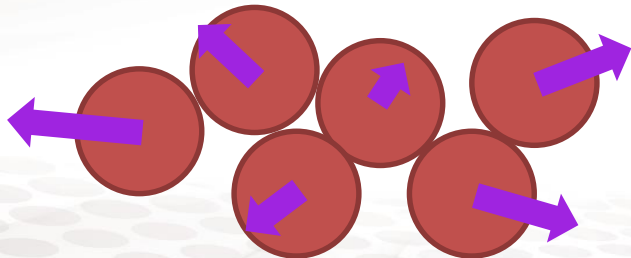
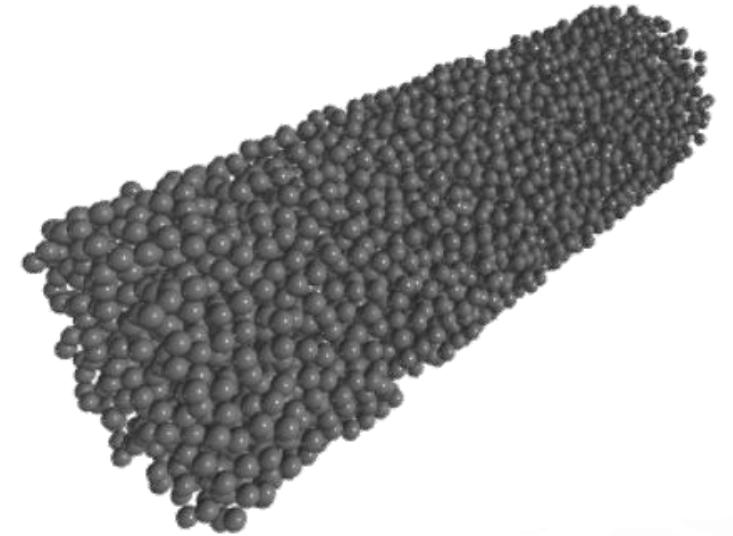
# Construction of a REV Shape cutting and adaptation



Particle selection

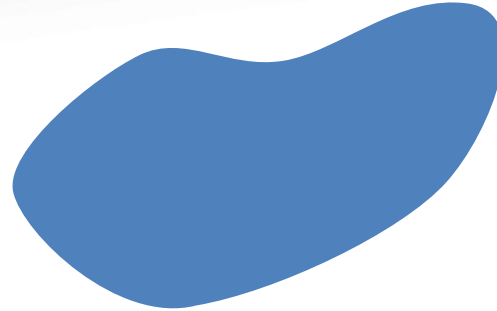


Implementation of the porosity and the proportion of alumina via an homothety.

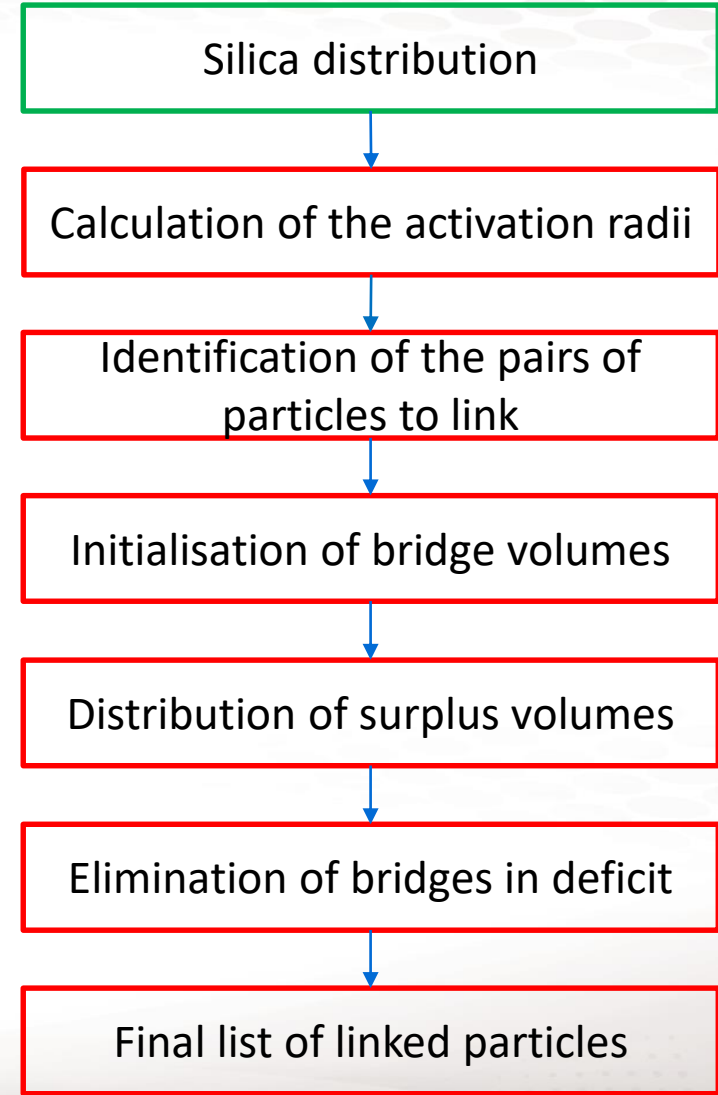
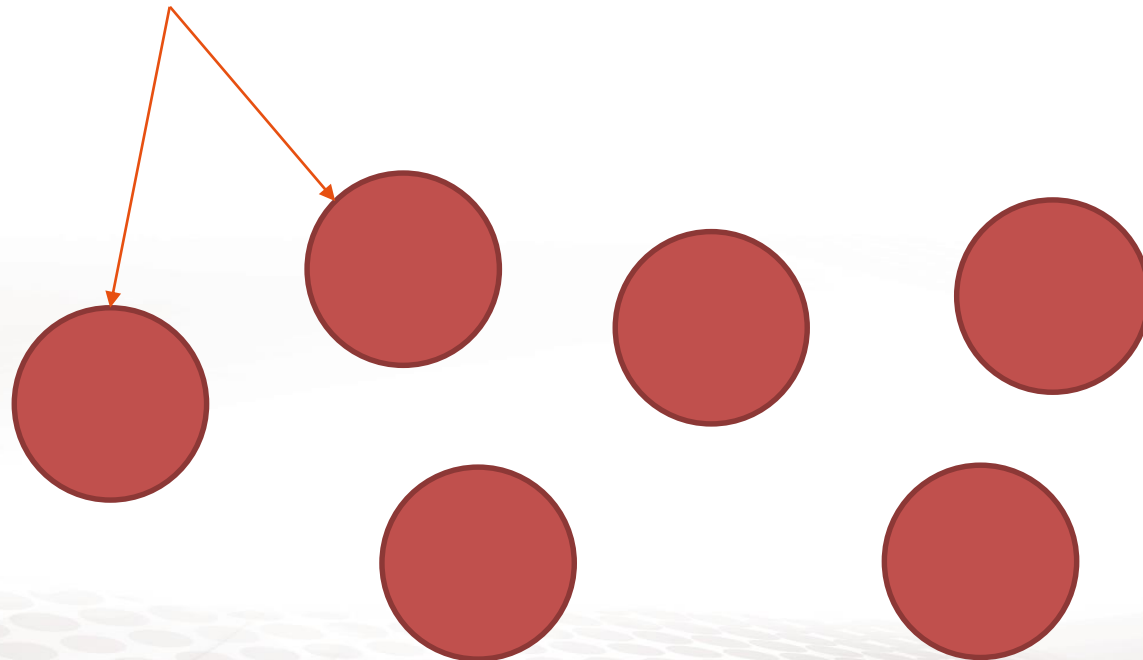


# Construction of a REV Formation of a lattice

Total silica quantity  
available in the REV



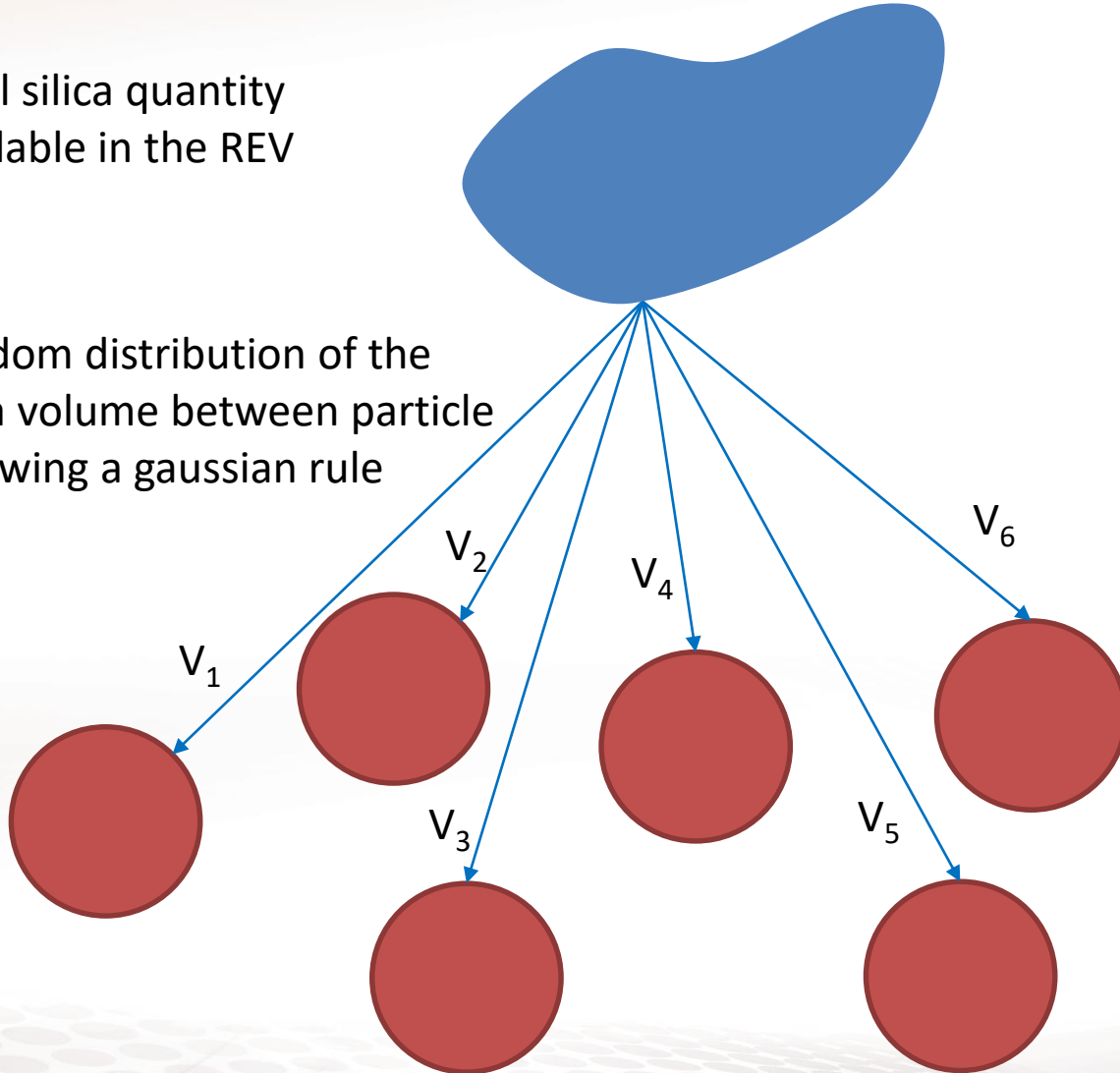
Alumina particle



# Construction of a REV Formation of a lattice

Total silica quantity available in the REV

Random distribution of the silica volume between particle following a gaussian rule

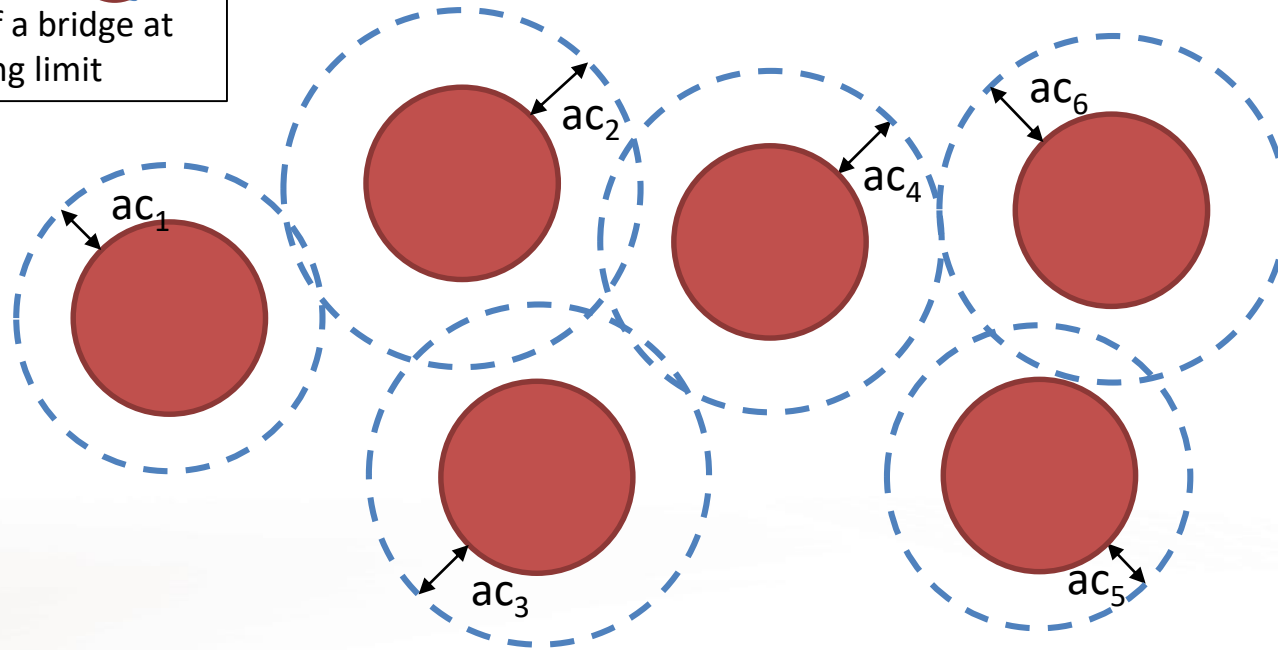
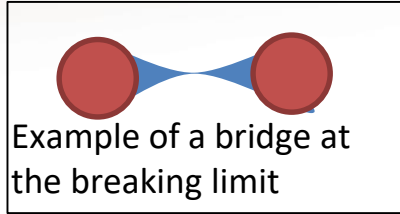


```

    graph TD
      A[Silica distribution] --> B[Calculation of the activation radii]
      B --> C[Identification of the pairs of particles to link]
      C --> D[Initialisation of bridge volumes]
      D --> E[Distribution of surplus volumes]
      E --> F[Elimination of bridges in deficit]
      F --> G[Final list of linked particles]
  
```

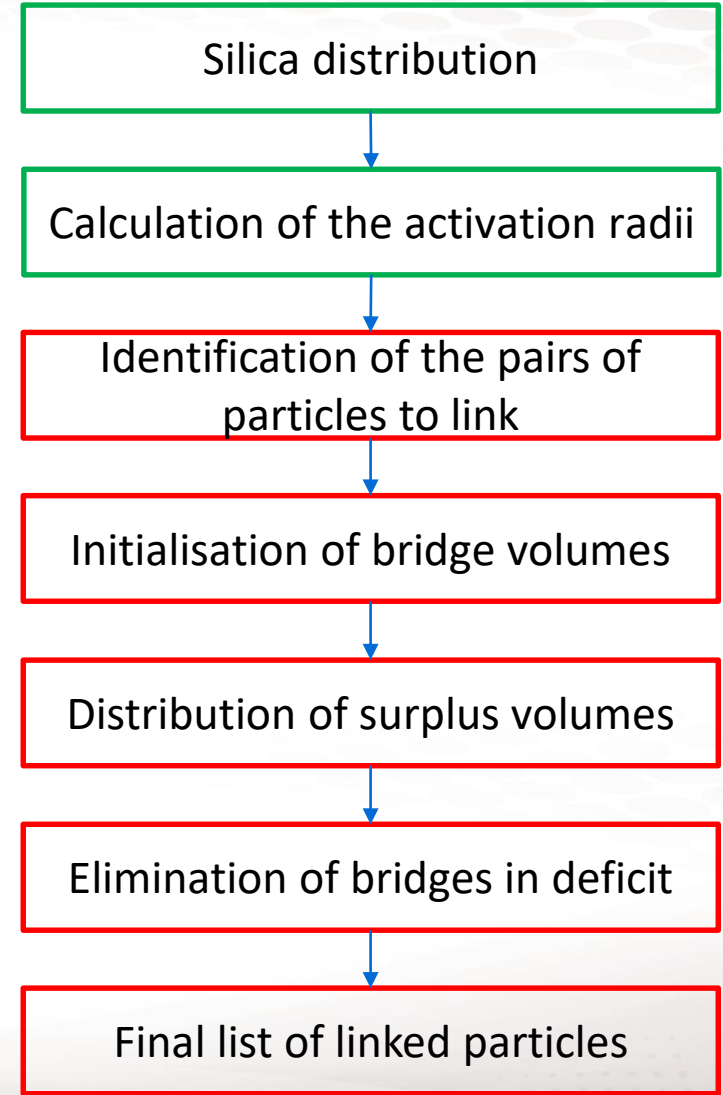


# Construction of a REV Formation of a lattice

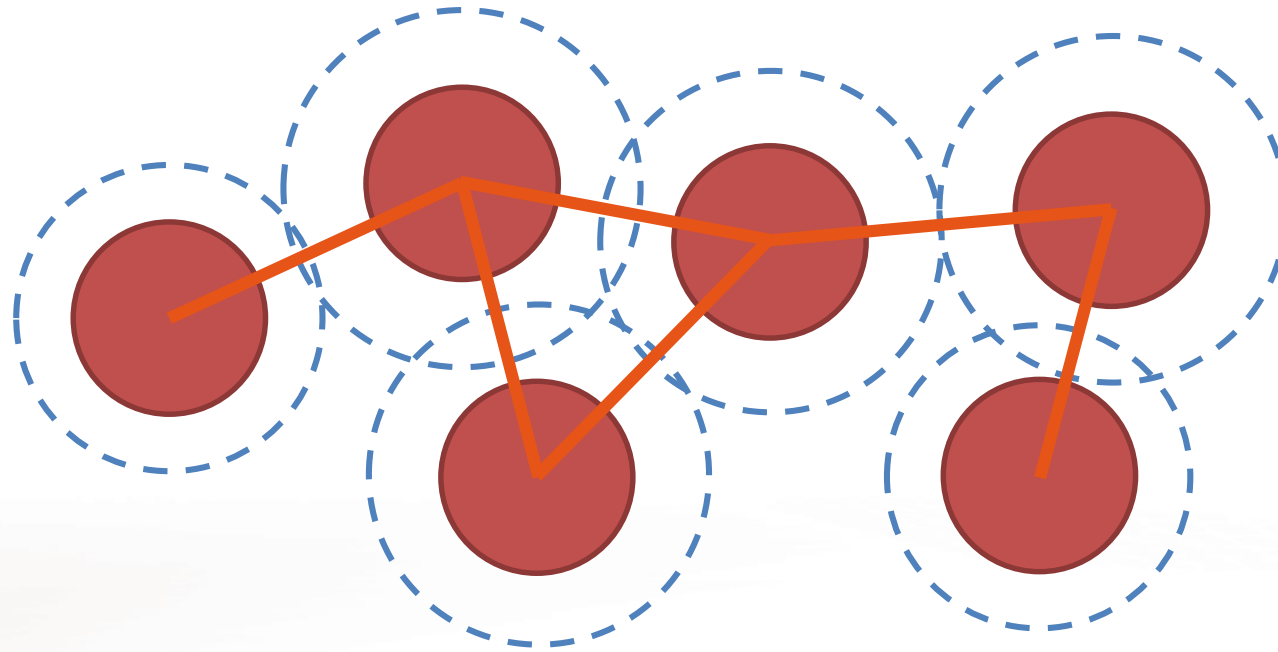


Activation radius definition :

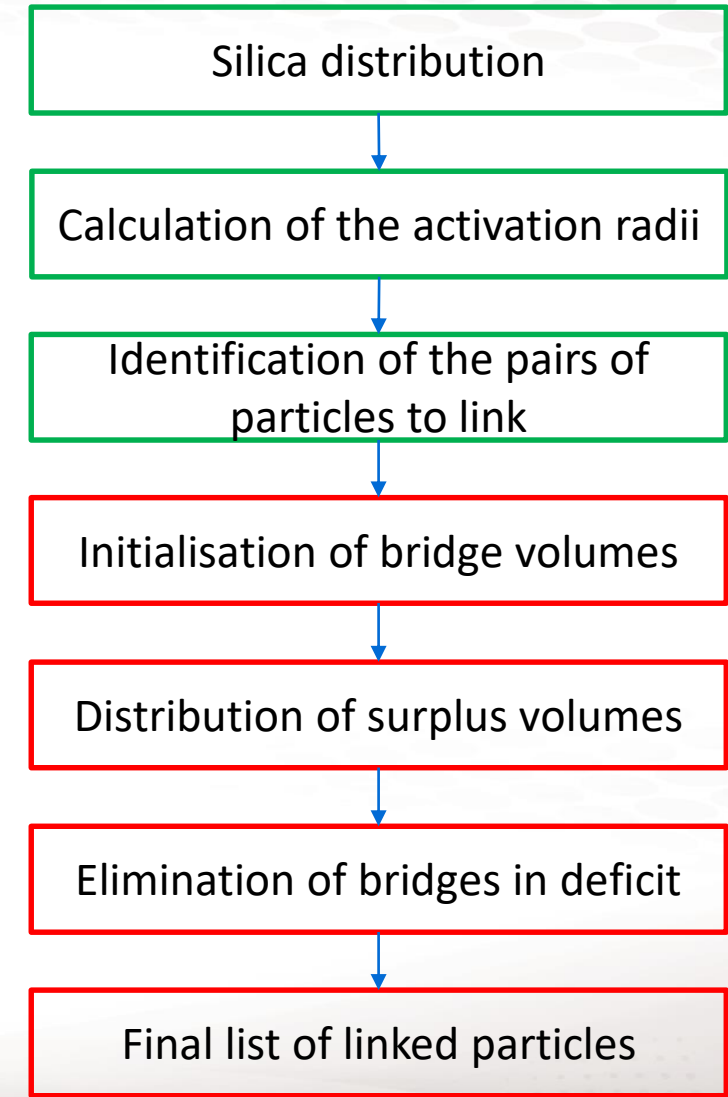
$ac$  : half distance of a bridge at the breaking limit associated to the silica volume given to the particle. ( $ac_i = \frac{1}{2} (1 + 0,5\delta) \sqrt[3]{V_i}$ )



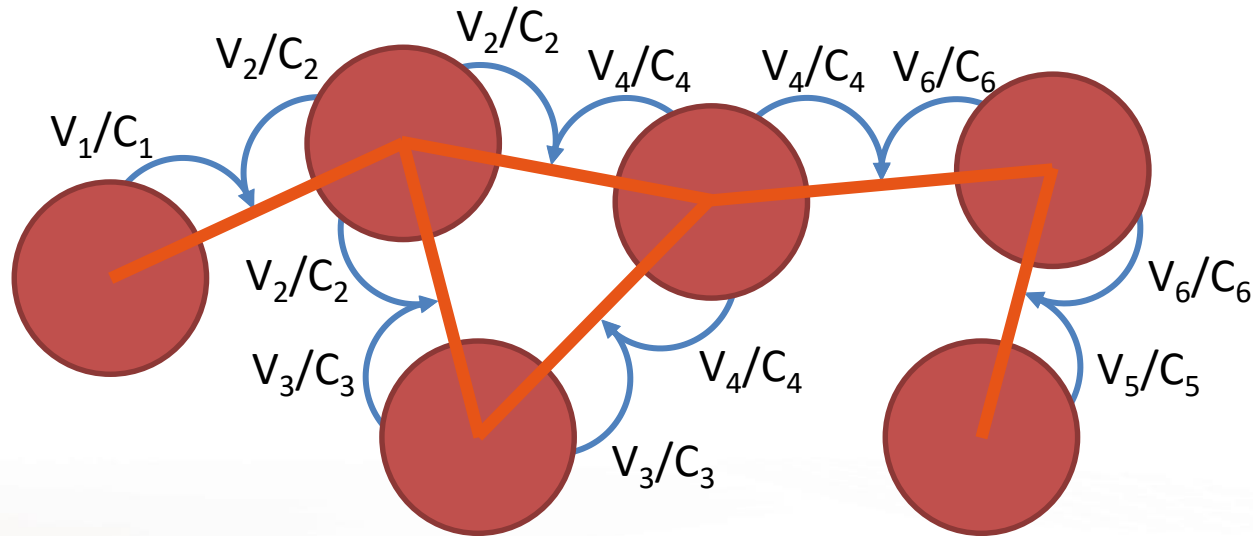
# Construction of a REV Formation of a lattice



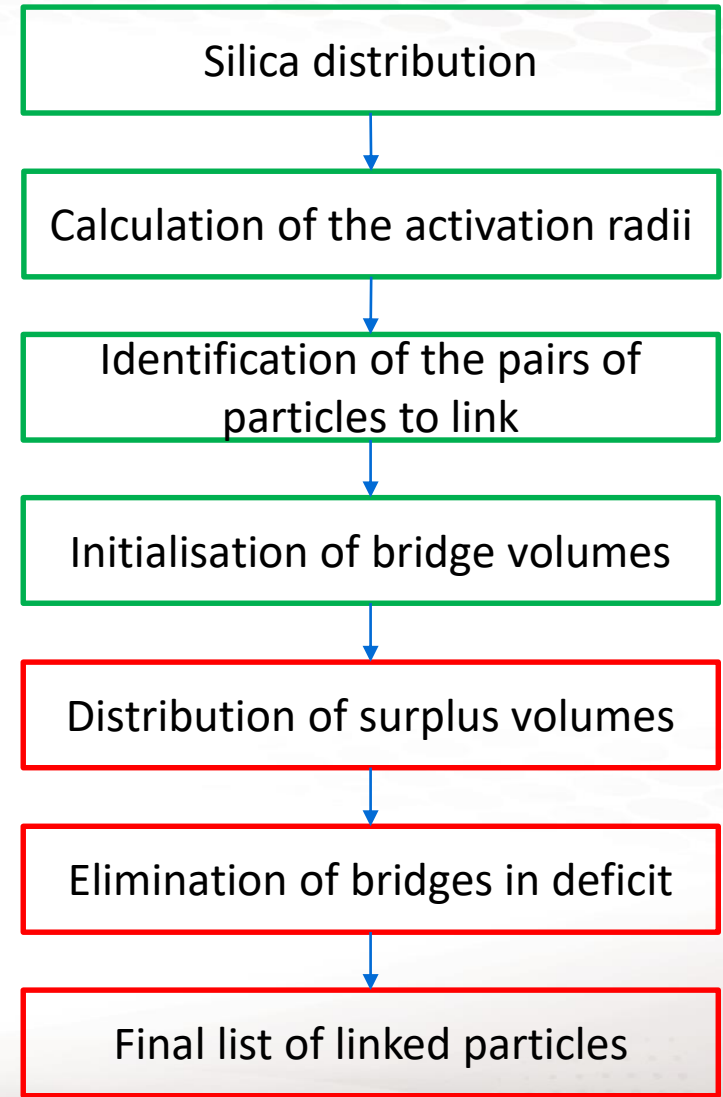
Initialisation of link between particle which activation radius intersect themselves.



# Construction of a REV Formation of a lattice

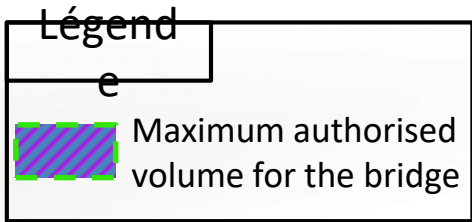
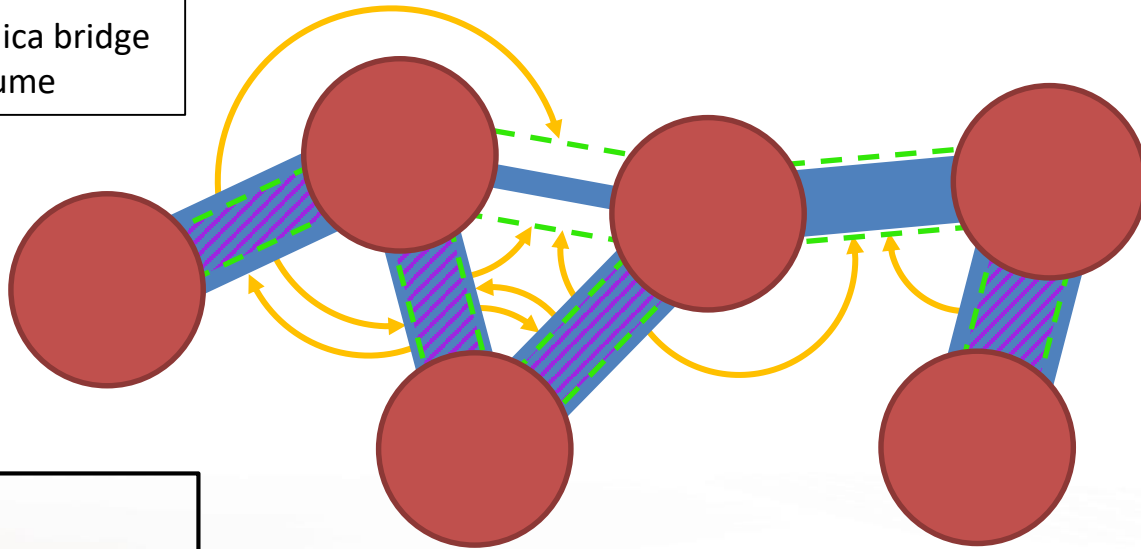
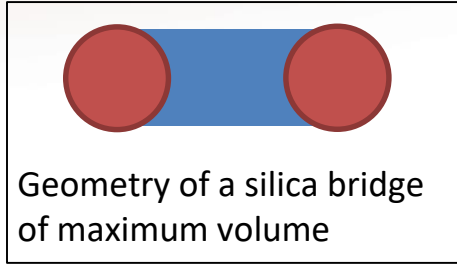


Allocation of a volume to each bond corresponding to the sum of the volume of silica allocated to the particle  $V_i$  divided by its coordinance  $C_i$ .

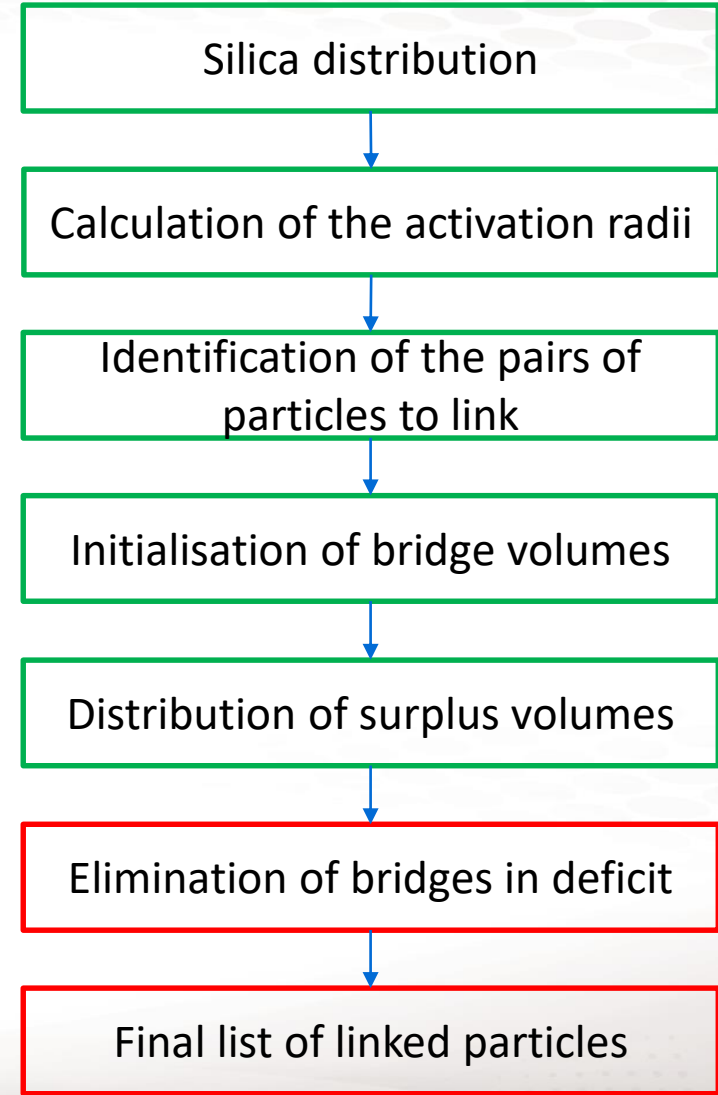




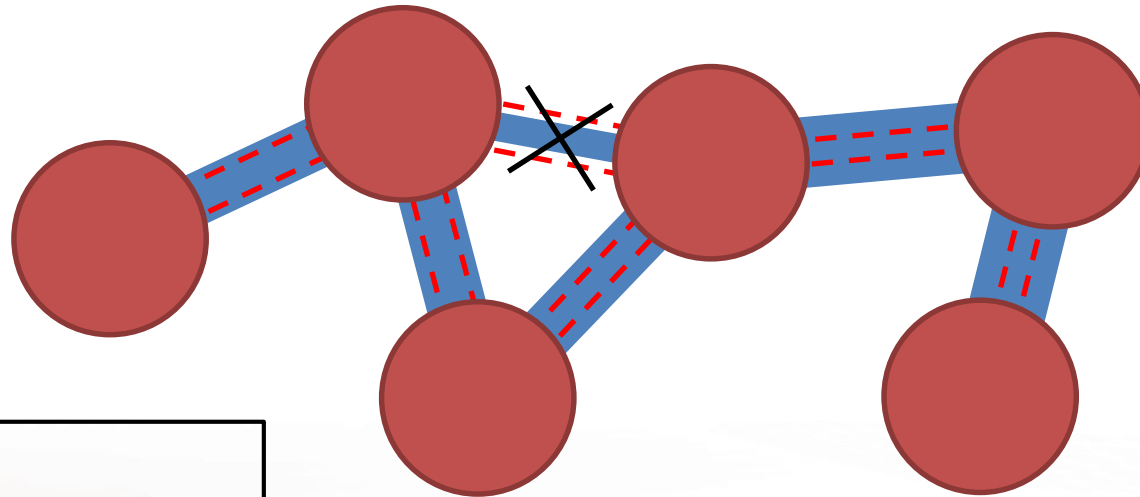
# Construction of a REV Formation of a lattice




The silica in bridges that are too large to be geometrically feasible is redistributed between neighbouring bridges.



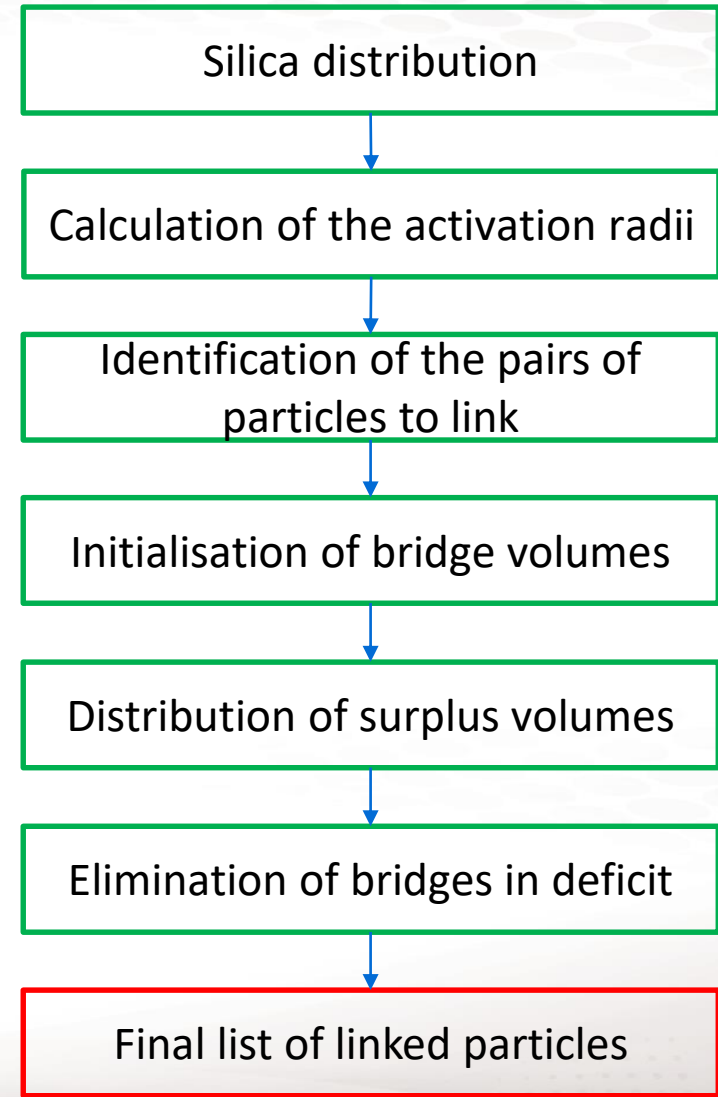
# Construction of a REV Formation of a lattice



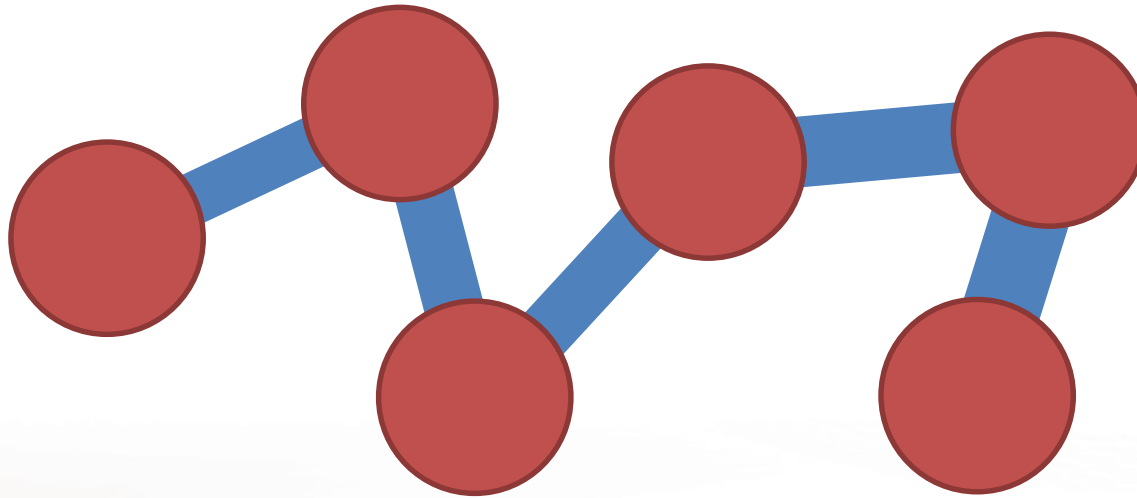
**Légende**

 Minimum volume authorised for the bridge

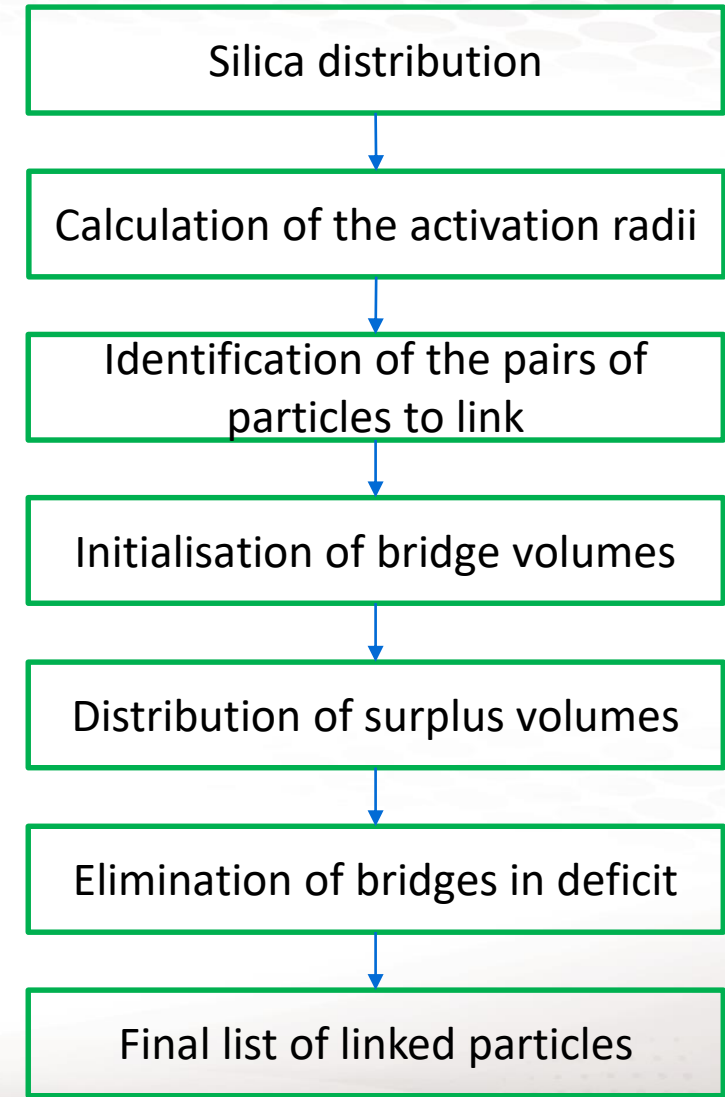
Bridges whose volumes are too low are eliminated from the lattice



# Construction of a REV Formation of a lattice

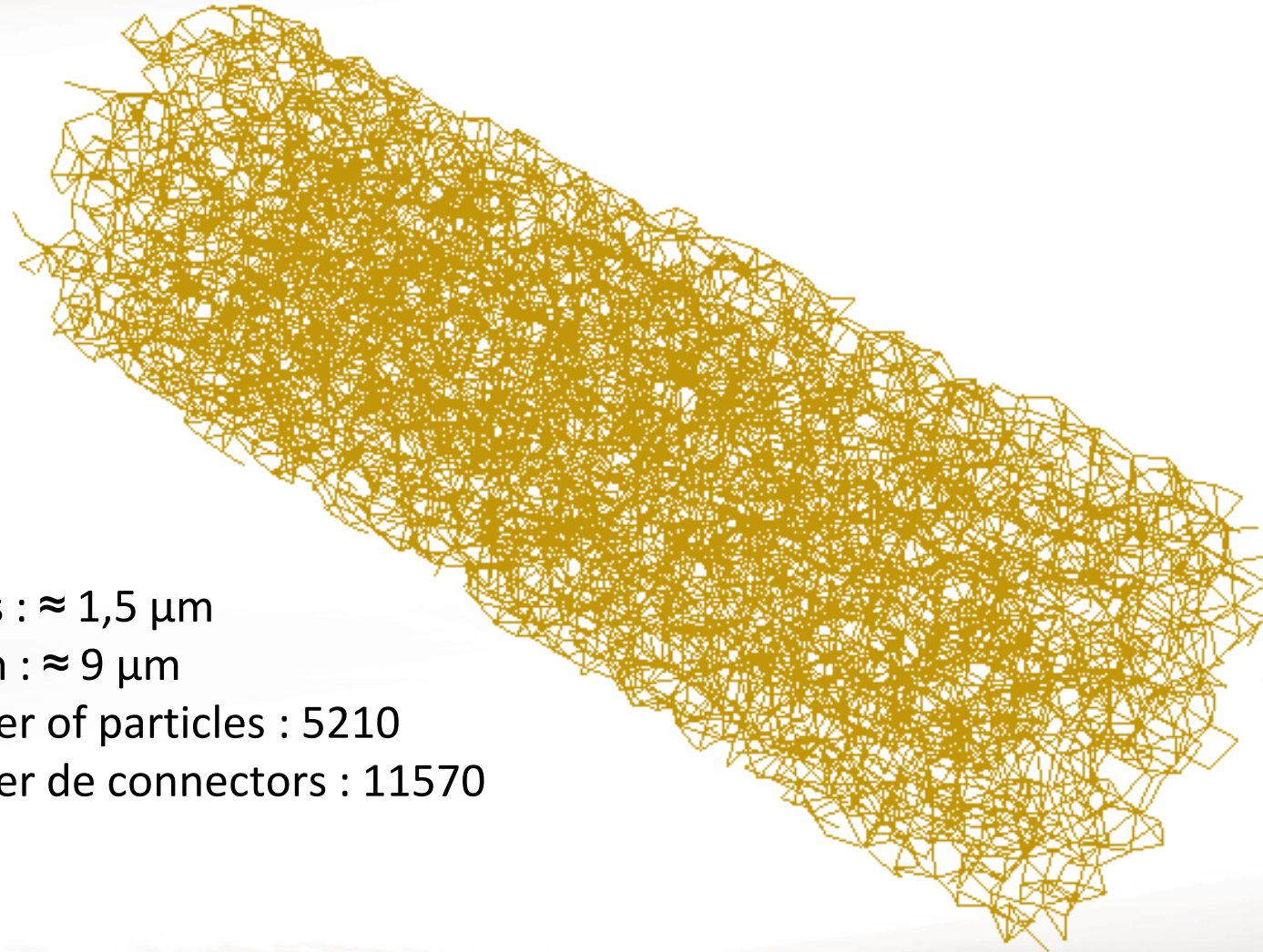


The lattice is formed and the rigidity of the bridges can be determined from their volume and length





# construction of a REV Example of a complete lattice



Radius :  $\approx 1,5 \mu\text{m}$

Length :  $\approx 9 \mu\text{m}$

Number of particles : 5210

Number de connectors : 11570

[1] : Walter Krenkel, Wiley-VCH Verlag GmbH&Co. KGaA. 2008.

[2] : F. W. Zok, *J American Ceramic Society*, vol. 89, n° 11, p. 3309-3324, nov. 2006

[3] : F. Boutenel, « Comportement d'une matrice alumine-silice au cours de l'élaboration de composites à matrice céramique oxyde/oxyde », thèse, novembre 2020.

[4] C. Ben Ramdane et al. *Journal of the European Ceramic Society*, vol. 37, no. 8, pp. 2919–2932, 2017.

[5] : Documentation Abaqus version 6,6 (section 25,1,5 connection-type library).