DE LA RECHERCHE À L'INDUSTRIE

Paris - Saclay

www.cea.fr

AMITEX_FFT training

-

General

-

V8.17.13

-

10/10/2023

L. Gélébart

OUTLOOK

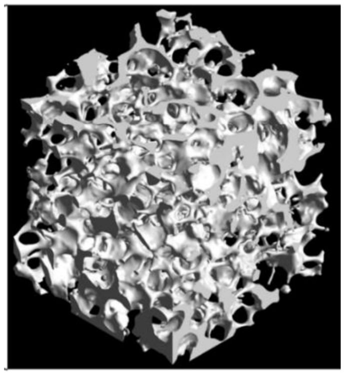
FFT-based methods

- General introduction
- AMITEX specificities
- Questions/answers in images

GENERAL INTRODUCTION

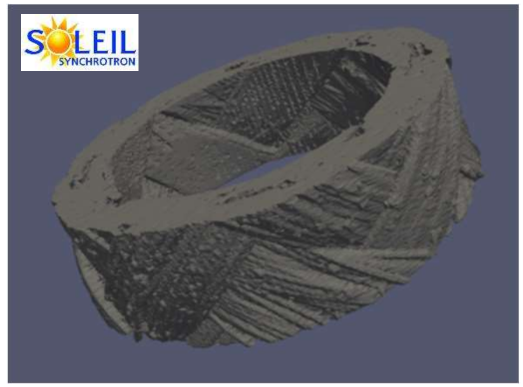
➢ Heterogeneous materials

❑ Porous ceramics



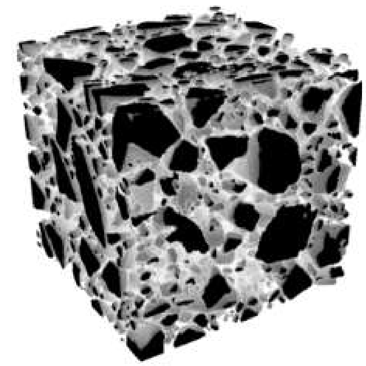
Ackermann &al. Materials 2014

❑ SiC/SiC composite tube



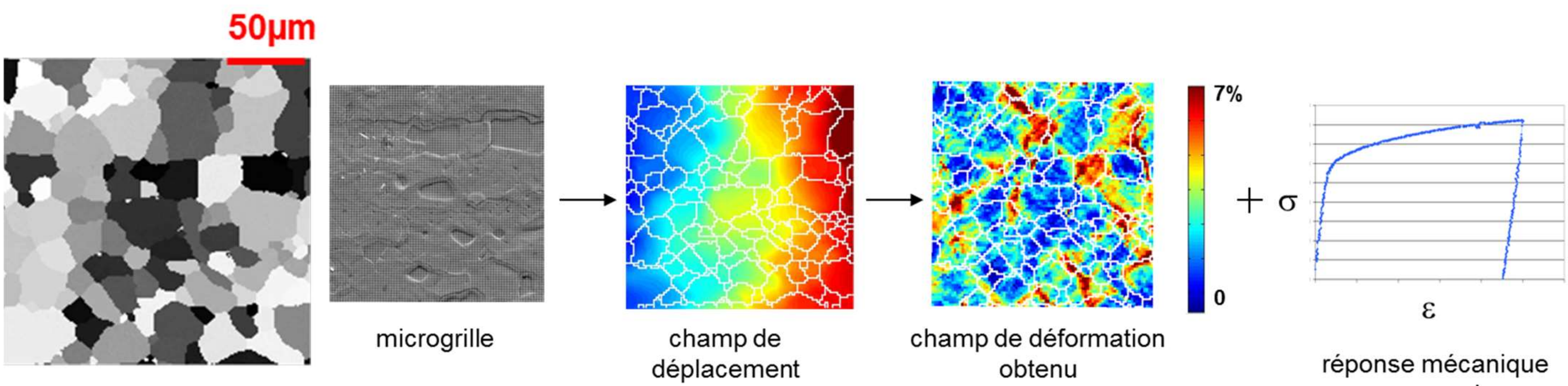
Thèse CHEN Y., CEA, ENPC, 2017

❑ Concrete



d'après F. Bernachy, CEA, 2017

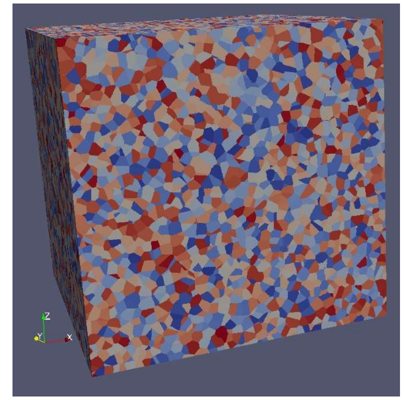
❑ Polycrystals



Thèse M. Dexet, CEA, LMS-X, 2006

GENERAL INTRODUCTION

➢ Simulation on Heterogeneous Materials



- **A « Representative » Volume Element**
- A **Behavior law** for each constituant
- An « **Average** » **loading :** uniaxial tensile test for example
- A type of Boundary Conditions **: Periodic**, often one of the best choice

➢ Natural Trends

- **Increase spatial resolution** (better description of local fields)
- **Increase the RVE size** (representativity for complex materials)
- More and more complex « **physically based** » **behaviors**
- ➢ Towards **non-local, multi-physics, code coupling**

➢ Standard FE solvers

- **Limits are rapidly reached (computation time and size)**

➢ « FFT » Solvers

- **Nos tedious meshing procedure**
- **More efficient than FE solvers**
- **Well-suited for parallelism => PUSH BACK THE LIMITS**

GENERAL INTRODUCTION

- **FIX-POINT algorithm on LIPPMAN-SCHWINGER (Moulinec-Suquet 1994)**

Problem to solve

$$\sigma(x) = c(x) : \varepsilon(x)$$
$$div(\sigma(x)) = 0$$
$$< \varepsilon(u(x)) >= E$$
$$+ \text{periodicity} + \text{compatibility}$$

$$\sigma(x) = c_0 : \varepsilon(x) + \underbrace{(c(x) - c_0) : \varepsilon(x))}_{\tau(x)}$$

Re-written problem

$$\sigma(x) = c_0 : \varepsilon(x) + \tau(x)$$
$$\tau(x) = (c(x) - c_0) : \varepsilon(x)$$
$$div(\sigma(x)) = 0$$
$$< \varepsilon(u(x)) >= E$$
$$+ \text{periodicity} + \text{compatibility}$$

Auxiliary probleme

$$\sigma(x) = c_0 : \varepsilon(x) + \tau(x)$$
$$div(\sigma(x)) = 0$$
$$< \varepsilon(u(x)) >= E$$
$$+ \text{periodicity} + \text{compatiblity}$$

Solution on auxiliary problem

$$\varepsilon(x) = -\Gamma_0 * \tau(x) + E$$

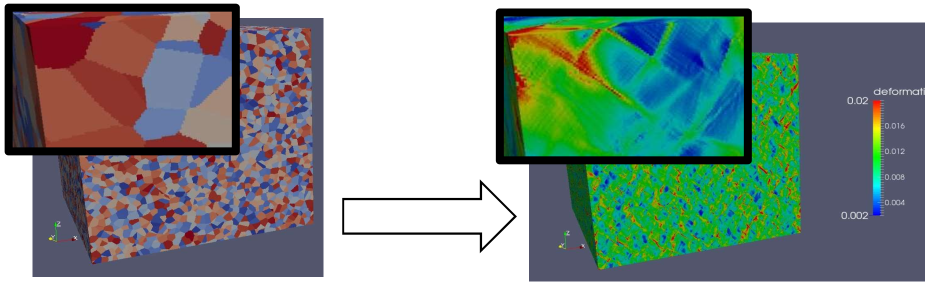
Applying the Green operator
Simple in Fourier space (FFT)
Mura 1997

Moulinec-Suquet,1994

$$\tau(x) = (c(x) - c_0) : \varepsilon(x)$$

DE LA RECHERCHE À L'INDUSTRIE

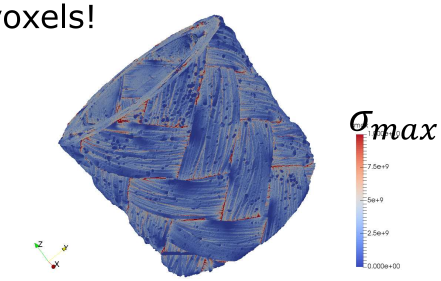
AMITEX_FFTP SPECIFICITIES



- **User interface**
- **Versatile**
- **Efficient**
- **Parallel**

- **Distributed Memory Implementation(MPI)**
  - **Models**
    - Mechanics Finite Strains
    - Mechanics Small Strains
    - Diffusion
  - **Algorithm**
    - Fix-Point + convergence algrithm
  - **Behavior**
    - umat compatibility => **mfront coupling!**
    - « Composite » voxels
  - **Various loadings**

7 Billion voxels!



AMITEX_FFTP SPECIFICITIES

➢ **Distributed Memory**

❑ Decomposition

✓ 1D Decomposition (slices)

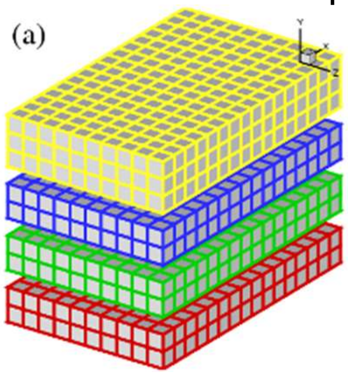


Image 1024^3

1024 processus max

Limiting for recent clusters!

✓ 2D Decomposition (pencils)

http://www.2decomp.org/

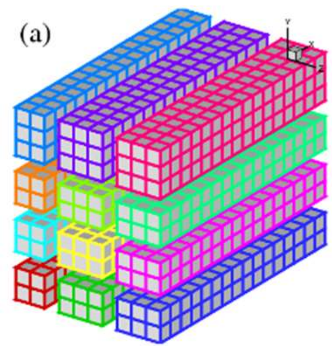


Image 1024^3

1024^2 processus max

Limit pushed back !

❑ Parallel resolution

➢ **'Classical' // solver** : **local per domain** + **interface domain**

➢ **FFT solver : directly on the whole domain** (in Fourier space)

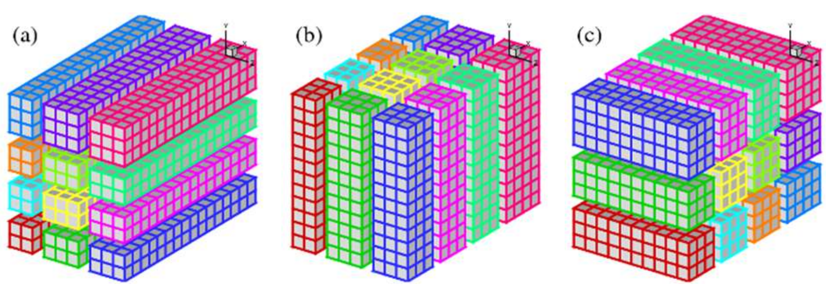
❑ FFT 3D = succession of 1D FFT

http://www.2decomp.org/

Requires data transposition

➢ Communications (MPI_ALLTOALL)!

➢ Librairie 2decomp



AMITEX_FFTP SPECIFICITIES

Cluster poincare (Maison de la Simulation)
16 cores (2x8) / node sandy bridge E5-2670

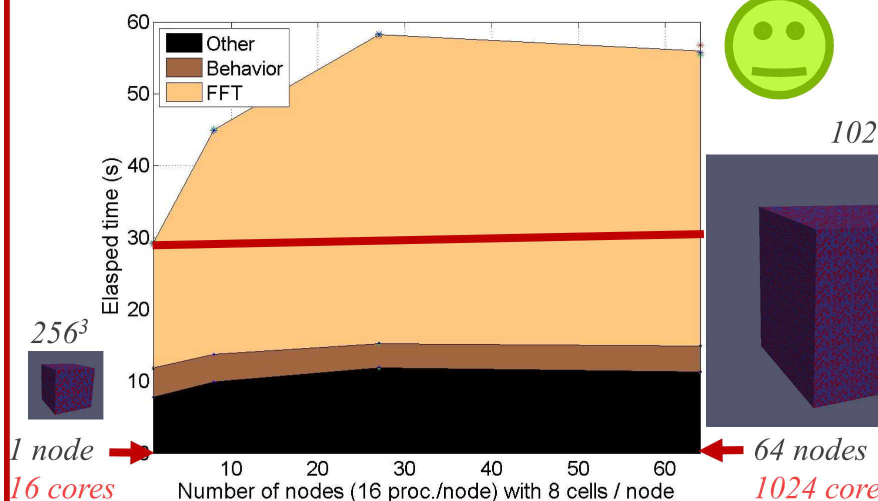
Scalability (weak)

Number of nodes= **N**, Pb size = **NxK0**

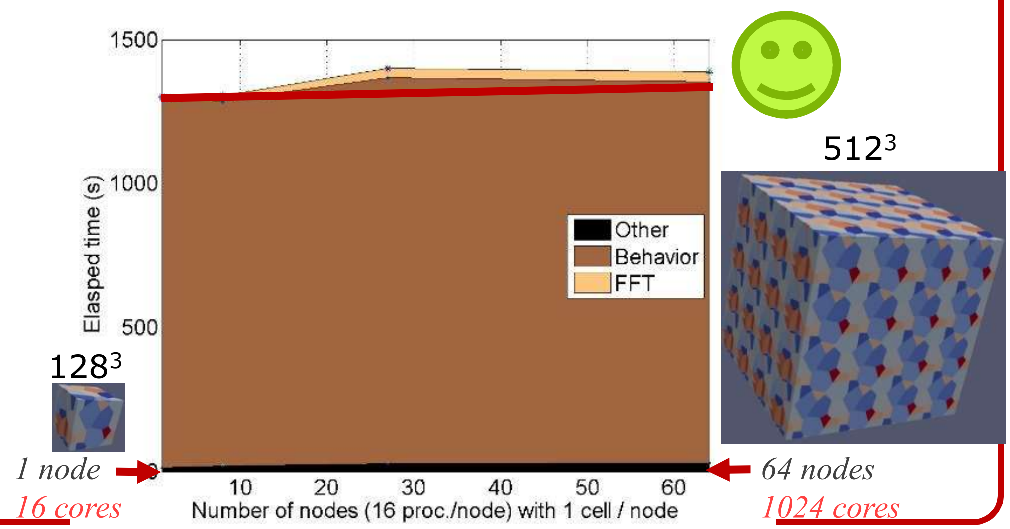
Time for N nodes : t_N

➢ Perfect scalability: $t_N = t_1$

"light behavior"
Elasticity



"heavy behavior"
Crystal plasticity



AMITEX_FFTP SPECIFICITES

➢ **Extension to Finite Strains**

❑ HPP

$$
\begin{cases}
div(\sigma) = 0 \\
\sigma = \sigma(\nabla u^{sym}) \\
u = \overline{\nabla u^{sym}}.x + u^{*} \\
u^{*}\ périodique \\
\sigma.n\ \#\ périodique
\end{cases}
$$

$$\tau = \sigma(\nabla u^{sym}) - c_0 : \nabla u^{sym}$$

$$\nabla u^{sym} = -\Gamma_0 * \tau + \overline{\nabla u^{sym}}$$

❑ Finite Strains

Initial configuration

$$
\begin{cases}
div(\pi) = 0 \\
\pi = \pi(\nabla u) \\
u = \overline{\nabla u}.X + u^{*} \\
u^{*}\ périodique \\
\pi.N\ \#\ périodique
\end{cases}
$$

$$\tau = \pi(\nabla u) - c_0 : \nabla u$$

$$\nabla u = -\Gamma_0^{GT} * \tau + \overline{\nabla u}$$

➢ IDENTICAL algorithms : UNIQUE implementation

$$\sigma \leftrightarrow \pi$$

$$\nabla u^{sym} \leftrightarrow \nabla u$$

$$\Gamma_0 \leftrightarrow \Gamma_0^{GT}$$

AMITEX_FFTP SPECIFICITIES

➢ **Convergence Acceleration (© CAST3M) on the FIX-POINT algorithm**

$$\tau^i = \sigma^i - C_0 : \varepsilon^i$$

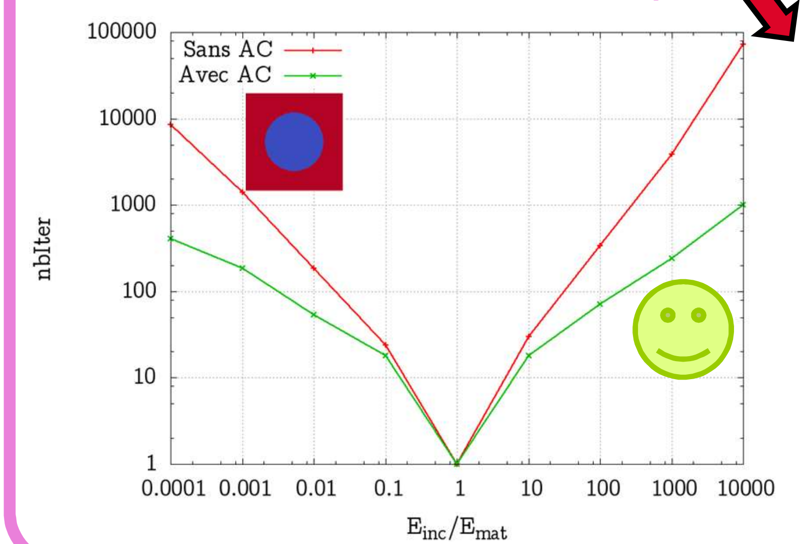
$$\varepsilon^{i+1} = -\Gamma_0 * \tau^i + E$$

$$\text{If } i + 1 \equiv 0[3] \quad \varepsilon^{i+1} = \sigma(\varepsilon^k, \varepsilon^{k+1} - \varepsilon^k \mid k = i, \dots, i-3)$$

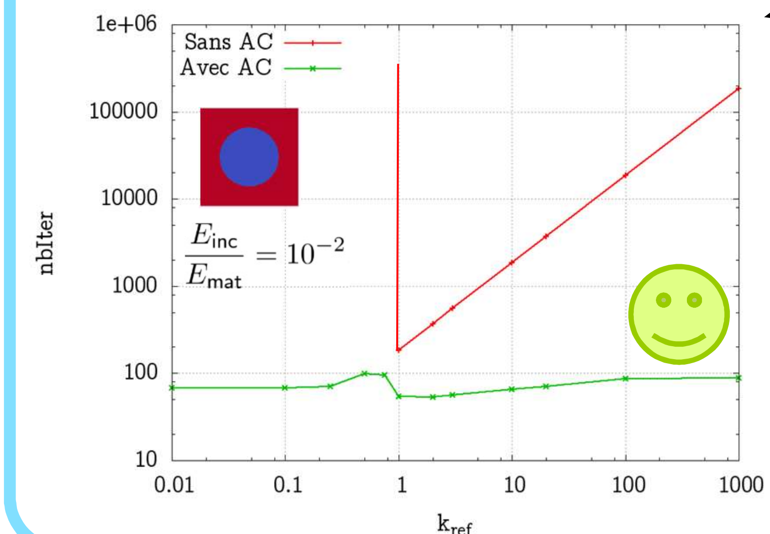
$$\sigma^{i+1} = c\left(\varepsilon^{i+1}\right)$$

- **Memory** : **4 couples** (Residual/Solution)
- **Efficiency!**
- No **tangent behavior** to evaluate!

Sensibilité au contraste mécanique



Sensibilité au Matériau de Référence

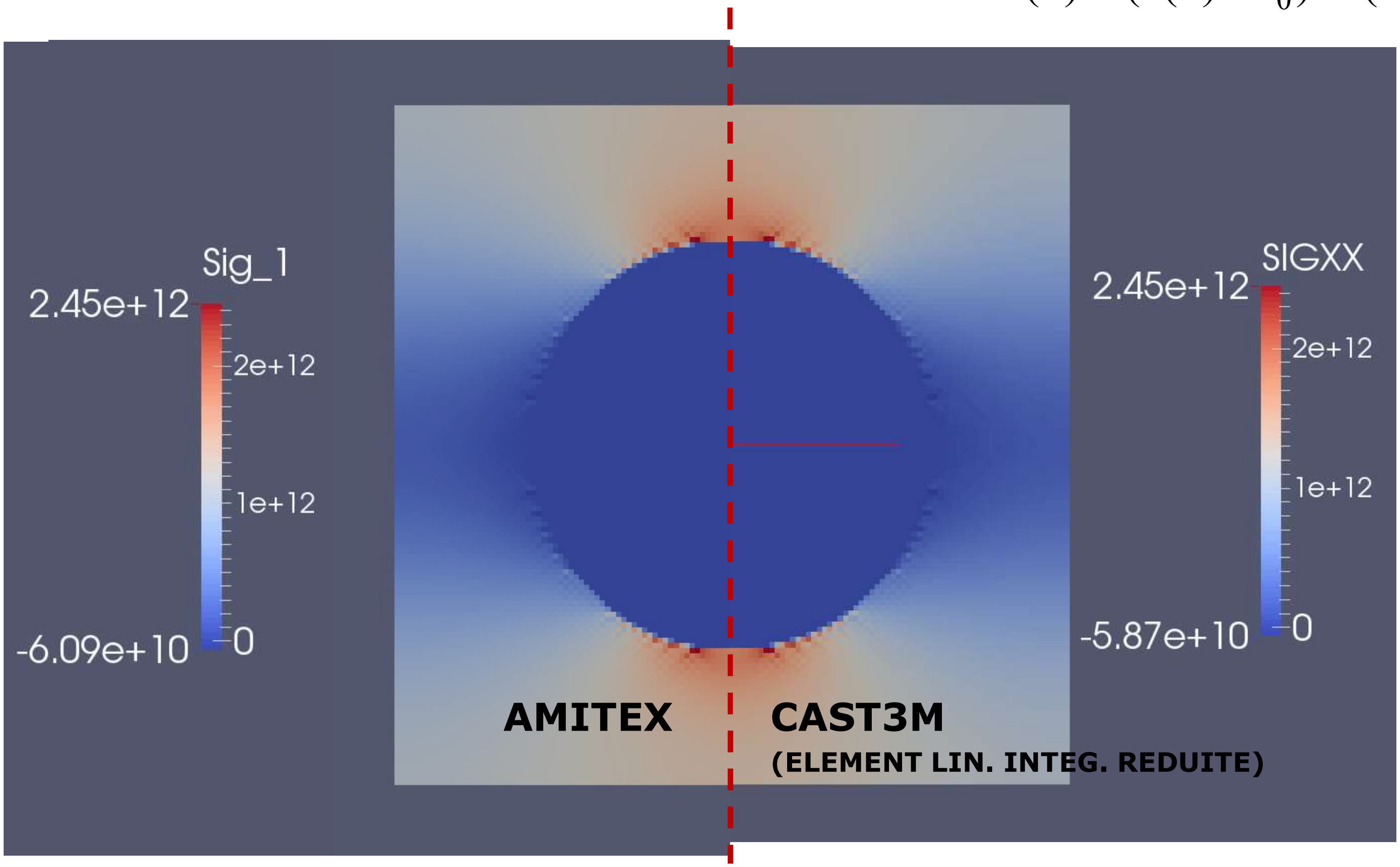


QUESTIONS – ANSWERS WITH IMAGES

- Difference with FE or Finite Differences? ➡ **Potentially* NONE**

* : if Green operator built on FE or DF discretization

$$\varepsilon(x) = -\Gamma_0 * \tau(x) + E$$
$$\tau(x) = (c(x) - c_0) : \varepsilon(x)$$

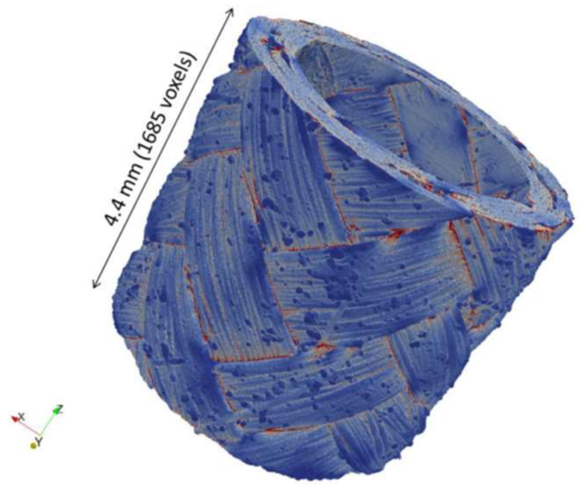


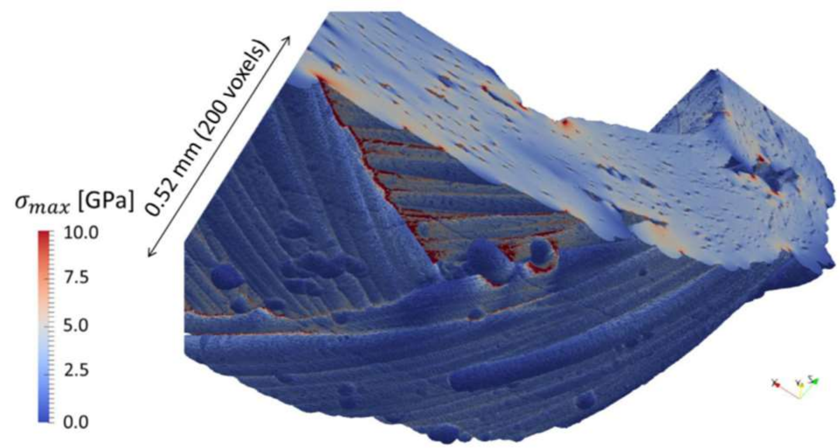
QUESTIONS – ANSWERS WITH IMAGES

- **Beyond Periodic Boundary Conditions ?** ➡ **YES**

Tensile test on SiC/SiC tube (tomo X)

Thèse Y. Chen

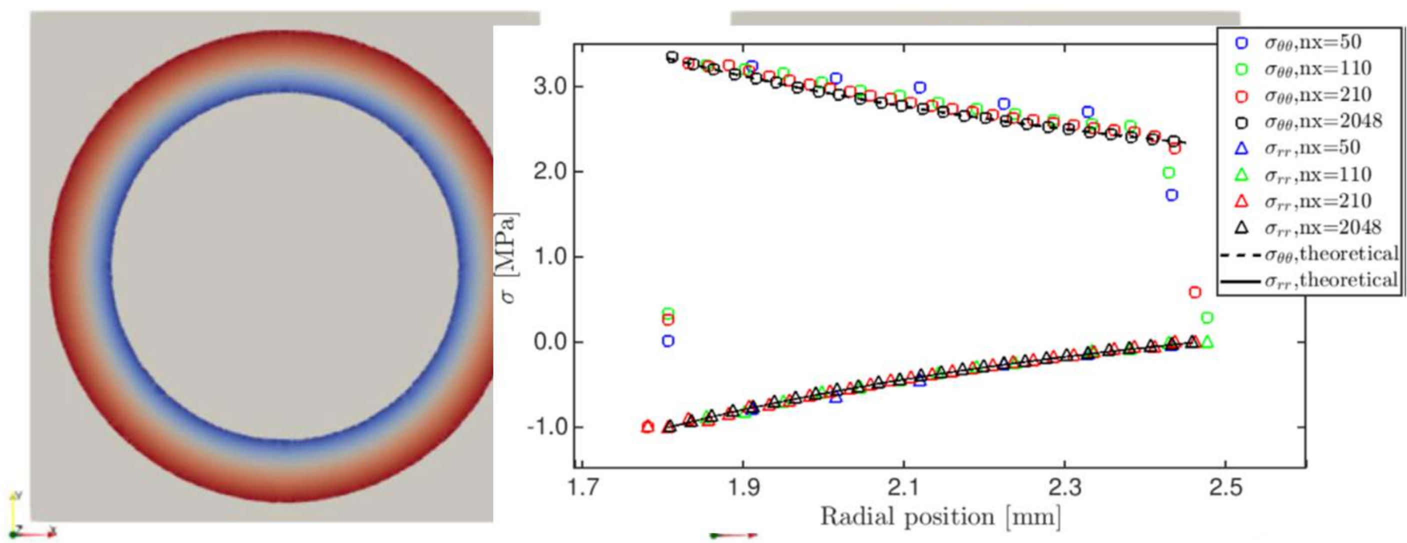




(b)

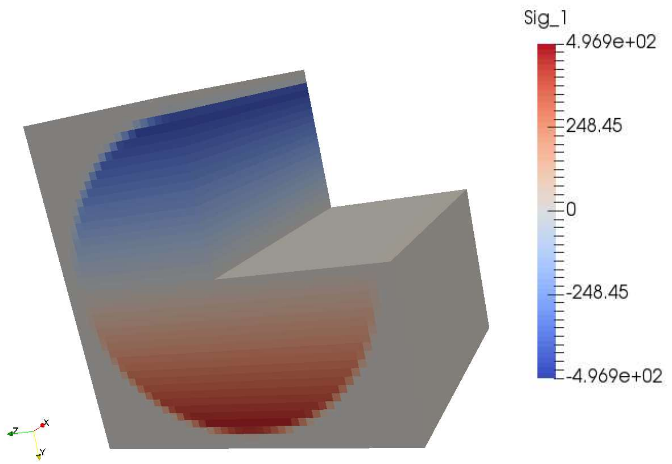
Internal pressure on a tube

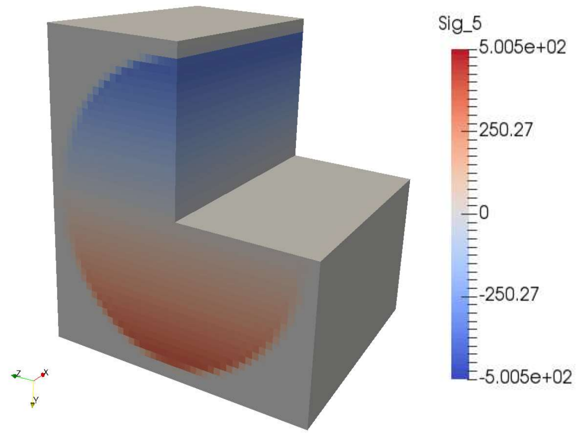
Thèse Y. Chen

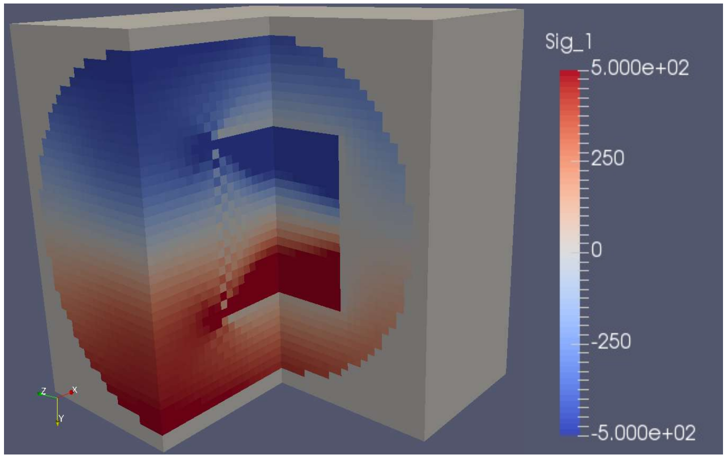


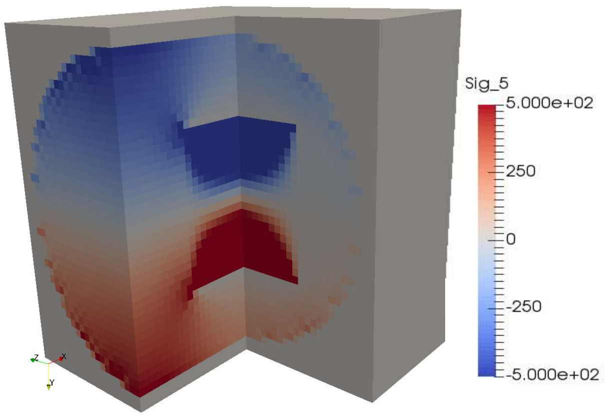
QUESTIONS – ANSWERS WITH IMAGES

- **And bending, torsion of beams and plates** ➡ **YES**







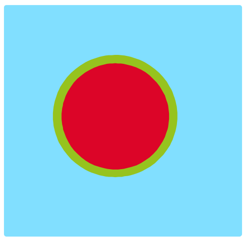


To be published…

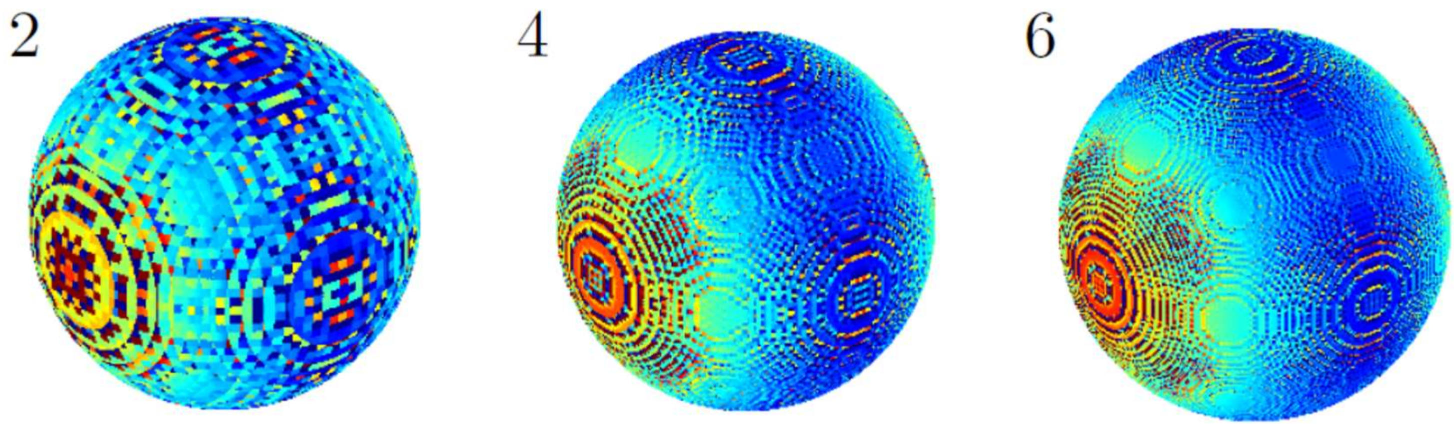
QUESTIONS – ANSWERS WITH IMAGES

- **Stresses at interfaces ?** ➡ **YES IF, composite voxels**

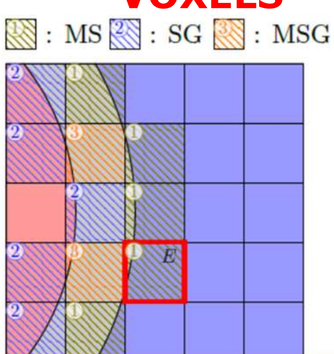
  ✓ Application to syntactic foam (PhD R. Charière)

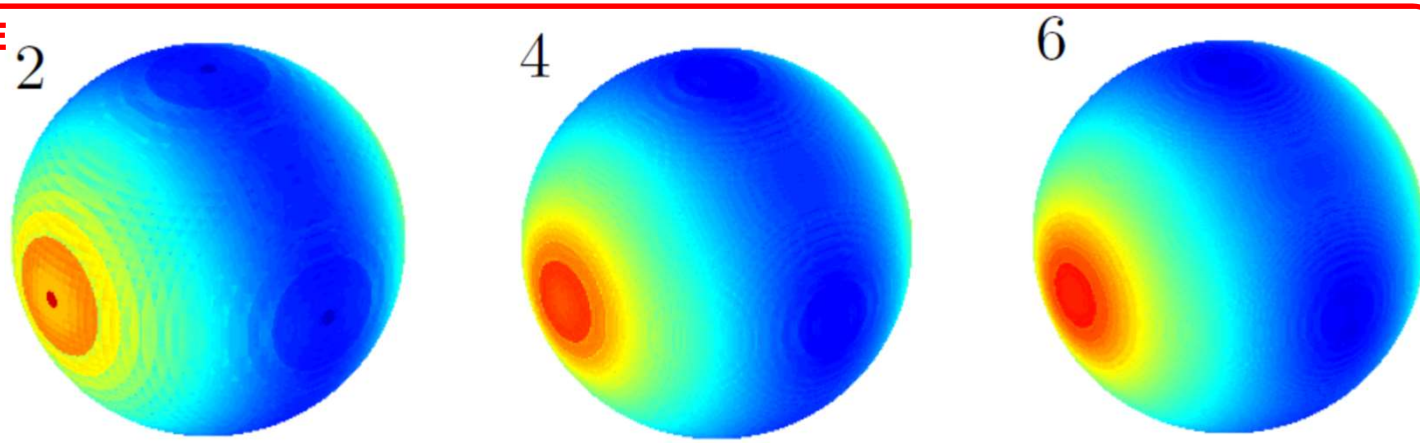


Evoid=0GPa
Eglass=69GPa
Epoly=1GPa



WITH COMPOSITE VOXELS

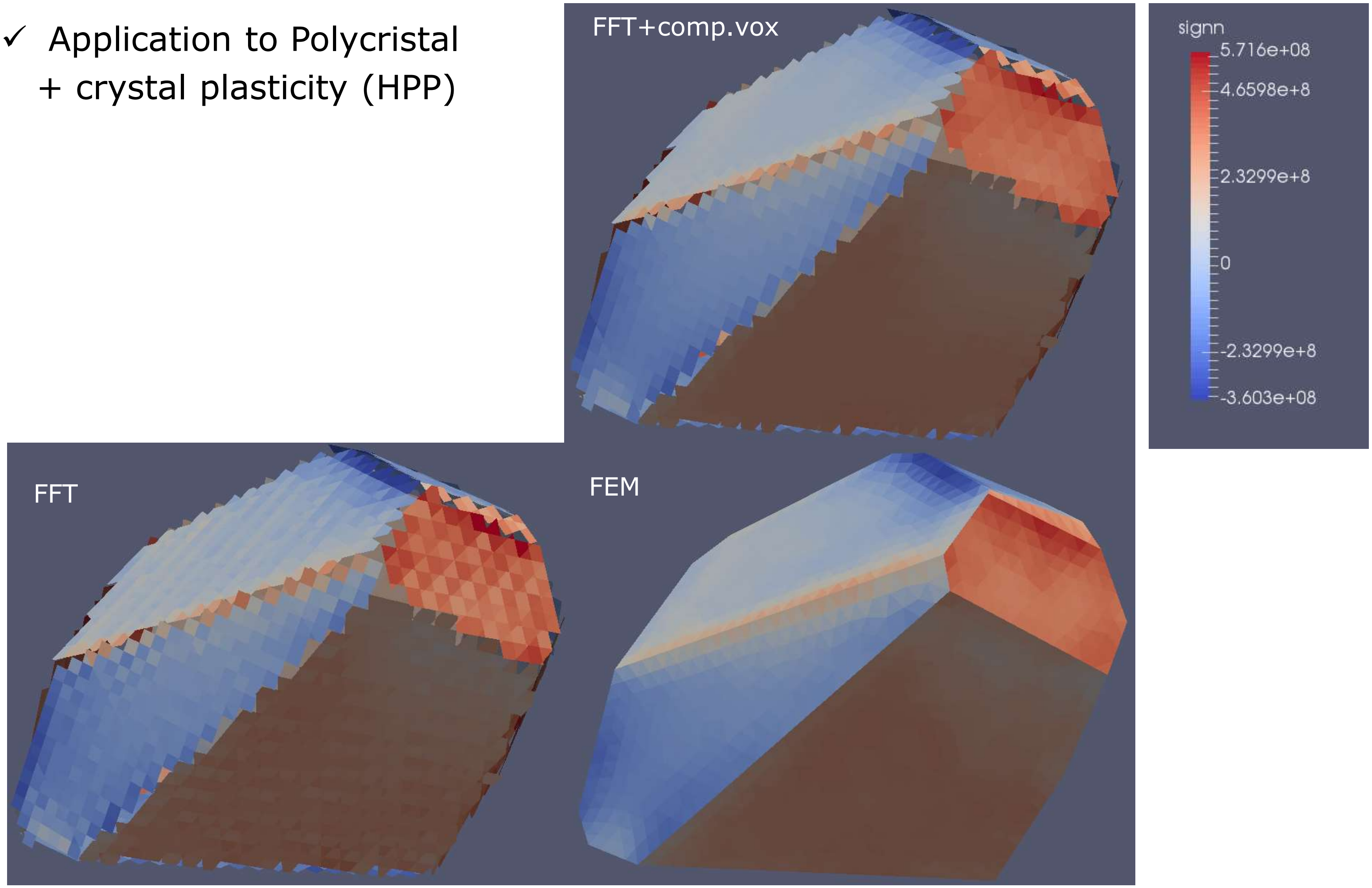




QUESTIONS – ANSWERS WITH IMAGES

- **Stresses at interfaces ?** ➡ **YES IF, composite voxels**

  ✓ Application to Polycristal
  + crystal plasticity (HPP)



VARIOUS QUESTIONS

Criteria

Average strain component	$\Rightarrow$	Exact (imposed)
Strain field compatibility	$\Rightarrow$	Exact (imposed)
Average stress component	$\Rightarrow$	Relative tolerance (default is 10^{-4})
Stress field equilibrium	$\Rightarrow$	Relative tolerance (default is 10^{-4})

Reference material Co ?

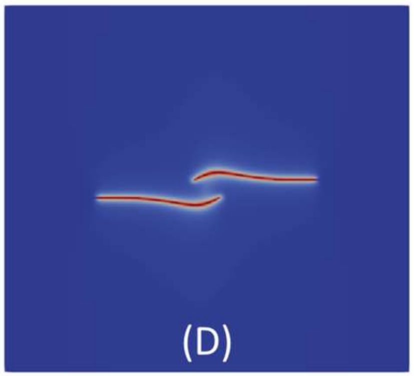
Convergence rate is affected by Co
With Convergence Acceleration the effect is lowered
A « good » choice for Co : Xo = (min(X)+max(X))/2 (with $X=\lambda$ or μ)
-> but in case of convergence issue, keep in mind that it can be optimized…

Solution (stress/strain fields) is not affected (up to the tolerance)

AMITEX « Extensions » for collaboration purpose

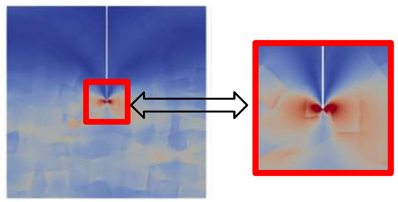
Various « Extensions » in progress…

Damage Phase Field

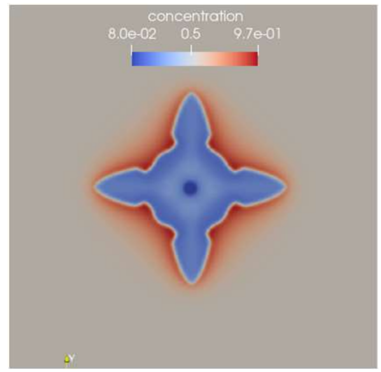


Collab. Y. Chen
(now @Bath Univ.)

Amitex Multi-Scale

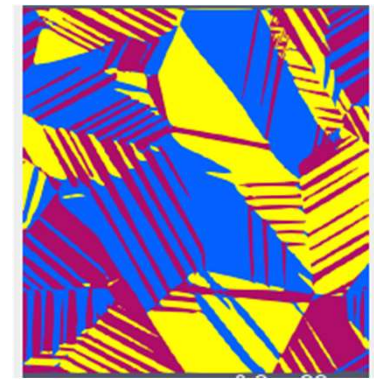


Solidification



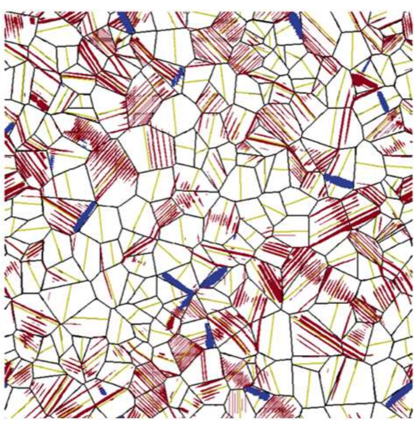
Collab, T. Pinomaa (VTT)

Solid Phase Transformation such as $\beta \rightarrow \alpha$ in Ti, Zr…

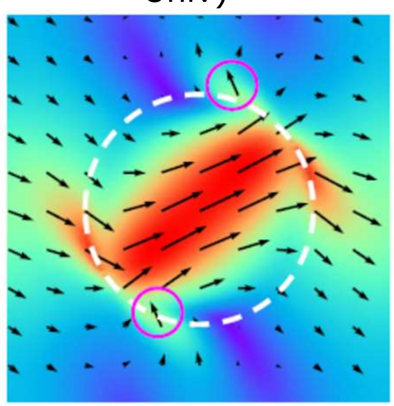


Collab J.Boisse
(LEMTA/ U. Lorraine)

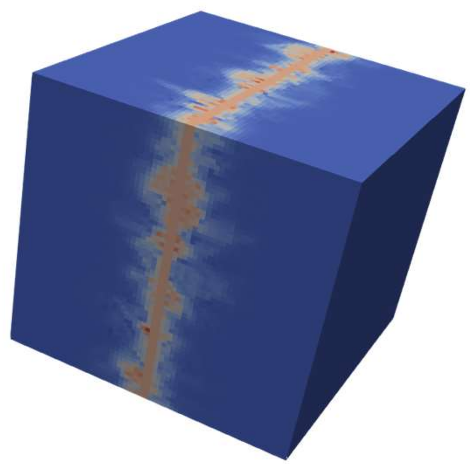
Non-local Crystal plasticity



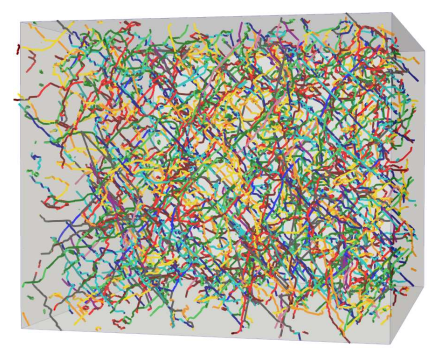
Flow in bi-porous media (Brinkman)
Y. Chen (Bath Univ)



Transient Thermal Simulations



DD coupling
Micromegas (ONERA)
Numodis (CEA – L. DUPUY)



ANNEXES

SPECIFICITES AMITEX_FFTP

➢ Parallélisme en mémoire distribuée (1)

$$\varepsilon^0(x) = E$$

$$\tau^k(x) = \sigma(\varepsilon^k(x)) - c_0 : \varepsilon^k(x)$$

$$\tau^k(x) \rightarrow \hat{\tau}^k(\xi)$$

$$\hat{\varepsilon}^{k+1}(\xi) = -\hat{\Gamma}_0(\xi) : \hat{\tau}^k(\xi) \qquad \hat{\varepsilon}^{k+1}(0) = E$$

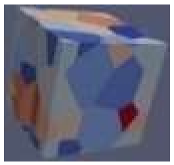
$$\hat{\varepsilon}^{k+1}(\xi) \rightarrow \varepsilon^{k+1}(x)$$

Parallélisme en mémoire distribuée (MPI)

- Comportement : « local » dans l'espace réel 
- Opérateur de Green : « local » dans l'espace de Fourier 
- FFT & iFFT : « non-local » 

SPECIFICITES AMITEX_FFTP

Scalabilité (2) : comportements « lourds »



- ✓ *Polycrystal (voronoï), **dislocation-based Crystal Plasticity (49 var.int.)**, HPP*
- ✓ *Cluster poincare (Maison de la Simulation)* 16 cores (2x8) / node sandy bridge E5-2670

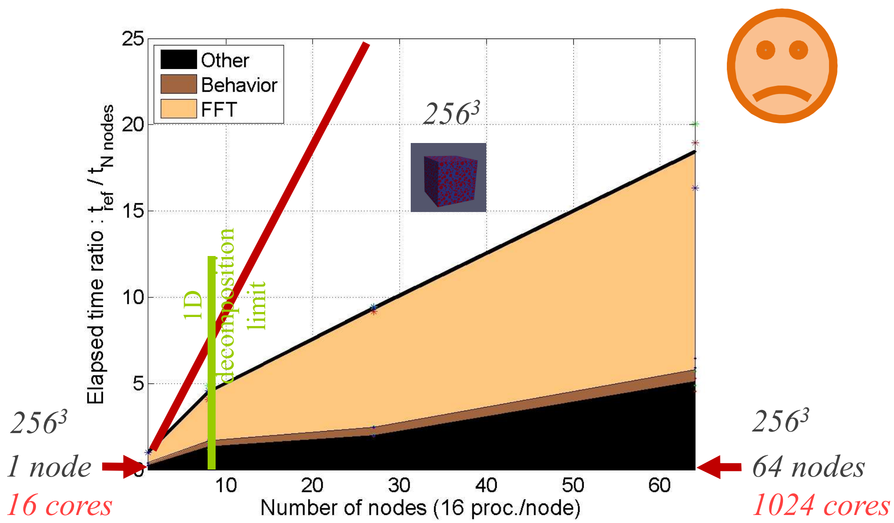
➢ Strong scalability

Number of nodes = **N**, Problem size = **K0**

Elapsed time on 1 node : t_{ref}

Elapsed time on N nodes : t_N

IDEALLY : $t_{ref} / t_N = N$



➢ Strong scalability

Number of nodes = **N**, Problem size = **K0**

Elapsed time on 1 node : t_{ref}

Elapsed time on N nodes : t_N

IDEALLY : $t_{ref} / t_N = N$