A massively parallel matrix free FE-based multigrid method for simulating the behavior of heterogeneous materials using large scale CT images

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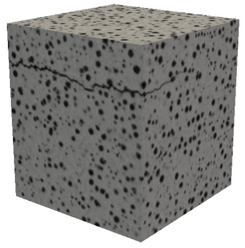
X-ray tomography opens new way to analyze materials

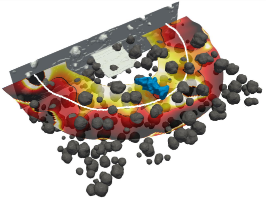
- 3D images μstructure (RVE) $\rightarrow$ computational homogenisation
- *in-situ* experiments
  - DVC: displacement / strain at the micro-scale

    microstructure $\leftrightarrow$ structure (geometry, BCs,...)
  - $\nearrow$ for crack / singularity

Crack in nodular graphite cast iron



PhD thesis J. Lachambre



Analysis of DVC fields

SIF, crack tip position,...

Background and motivations

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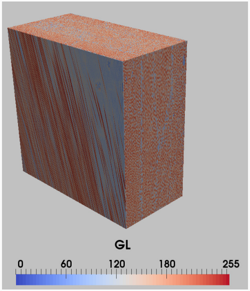
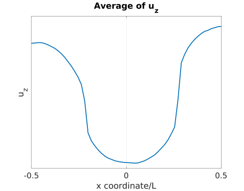
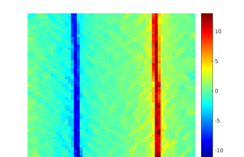
Laminate composite material



Averaged U_Z on the free surface



Strain_{XZ} on the free surface



Lecomte-Grosbras, P., *et al.*. Experimental Mechanics, 2015.

Background and motivations

X-ray tomography opens new way to analyze materials

- 3D images μstructure (RVE) $\rightarrow$ computational homogenisation
- *in-situ* experiments
  - DVC: displacement / strain at the micro-scale

    microstructure $\leftrightarrow$ structure (geometry, BCs,...)
  - $\nearrow$ for crack / singularity

Usually DVC results are difficult to analyse / interpret

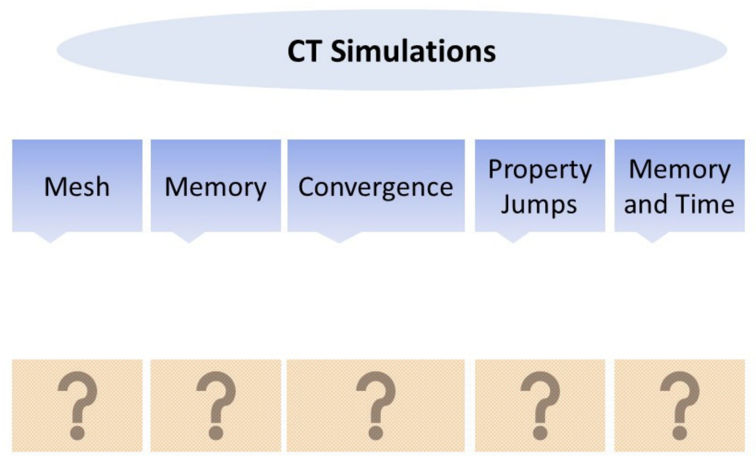
- microstructure $\leftrightarrow$ structure
- DVC (spatial-)resolution $\approx$ a few tens of voxels
- neither a micro displacement nor a macro displacement

$\rightarrow$ need to perform numerical simulations at the micro-scale to

- understand these interactions
- analyse the DVC results

Objective & questions

Perform **automatically** numerical simulations using **large CT** images, *e.g.* 8 billion voxels, of **heterogeneous** materials.



Well-known numerical methods:

- Finite Element Methods (FEM): (LENGSFELD *et al.* 1998, FERRANT *et al.* 1999)
- Fast Fourier Transform (FFT): (NEMAT-NASSER *et al.* 1982, SUQUET 1990)
- Finite Difference Methods (FDM): (GU *et al.* 2016)

LENGSFELD M., SCHMITT J., ALTER P., KAMINSKY J., LEPPEK R., Medical engineering & physics, 20, 515-522, 1998.
FERRANT M., WARFIELD S. K., GUTTMANN C. R., MULKERN R. V., JOLESZ F. A., KIKINIS R., International Conference on Medical Image Computing and Computer-Assisted Intervention Springer, 202-209, 1999
NEMAT-NASSER S., IWAKUMA T., HEJAZI M., Mechanics of materials, 1, 239-267, 1982.
SUQUET P., Comptes rendus de l'Académie des sciences. Série 2, Mécanique, Physique, Chimie, Sciences de l'univers, Sciences de la Terre,311, 769-774, 1990.
Gu, H., Réthoré, J., Baietto, M.-C., Sainsot, P., Lecomte-Grosbras, P., Venner, C. H., Lubrecht, A. A., Computational materials science, 112, 230-237, 2016

State of the art

Advantages of each numerical method for large scale CT simulations:

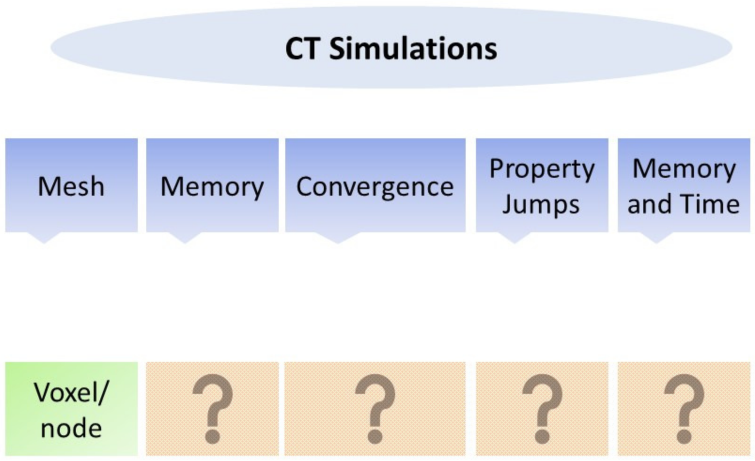
- FEM:
  - Abundant element types can deal with complex geometry
  - Implementation of boundary conditions is straightforward
- FFT:
  - Performed on the regular voxel grid
  - Efficient for **periodic** problems
- FDM:
  - Mesh generation is efficient (one voxel/point)
  - Smaller memory requirement

Drawbacks of each numerical method for large scale CT simulations:

- FEM: expensive on **Meshing** step and **relaxation** step
- FFT: only for **periodic** boundary condition problems
- FDM: boundary conditions are difficult to implement

Proposed strategy

FEM with one node = one voxel



Thermal conduction in heterogeneous materials:

$$\begin{cases} \nabla \cdot (\boldsymbol{\alpha} \nabla T) = 0 & \\ T = T_0 & \text{on } \Gamma_1 \\ T = T_1 & \text{on } \Gamma_2 \\ \boldsymbol{\alpha} \cdot \nabla T \cdot \boldsymbol{n} = 0 & \text{on the other surfaces} \end{cases}$$

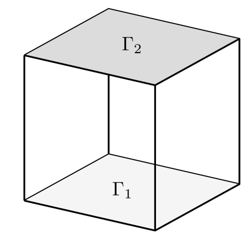


Figure 1: Boundary conditions

- $\boldsymbol{\alpha}$ is a high contrast variable coefficient (1∼1 000)

FEM

The weak form of the original equation:

$$-\int_{\partial\Omega} \boldsymbol{\alpha}\nabla T \cdot \vec{n}\varphi \, dS + \int_{\Omega} \boldsymbol{\alpha}\nabla T \cdot \nabla\varphi \, d\Omega = 0$$

which is also referred to: $\mathsf{q}_{\mathsf{in}} = \mathsf{q}_{\mathsf{ex}}$ with

$$\begin{cases} \mathsf{q}_{\mathsf{in}} = & -\int_{\Omega} \boldsymbol{\alpha}\nabla T \cdot \nabla\varphi \, d\Omega \\ \mathsf{q}_{\mathsf{ex}} = & -\int_{\partial\Omega} \boldsymbol{\alpha}\nabla T \cdot \vec{n}\varphi \, dS \end{cases}$$

One voxel per elementary node, at node j with MF-FEM:

$$(q_{in})_j = -\sum_e \sum_i \sum_m \sum_{g=1}^{8} w_g \nabla_m \varphi_i \alpha^g T_i \nabla_m \varphi_j$$

α^g is the conductivity at Gauss integration point:

$$\alpha^g = \sum_{i=1}^{8} \alpha_i \varphi_i$$

Jacobi relaxation node by node without matrix assembly:

$$T_i^{iter+1} = T_i^{iter} + \omega \frac{(q_{ex} - q_{in})_i}{stiff_i}$$

ω: relaxation coefficient.

$$stiff_i = \sum_e \sum_m \sum_{g=1}^{8} w_g \nabla_m \varphi_i \alpha^g \nabla_m \varphi_i$$

Matrix free FEM (MF-FEM) (HUGHES *et al.* 1983):

- Dispenses from assembling stiffness matrix: Size of stiffness matrix (sparse):3.8 TB for a problem with 18 billion of DoF
- Suited for voxel conversion problems (one element type)

HUGHES T. J., LEVIT I., WINGET J. Computer Methods in Applied Mechanics and Engineering, 36(2), 241–254, 1983.

Performance of MF-FEM

Proposed Jacobi MF-FEM for a 129^3 nodes spherical thermal conduction problem with a contrast of 10

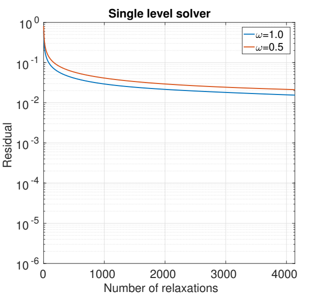


Figure 2: Convergence

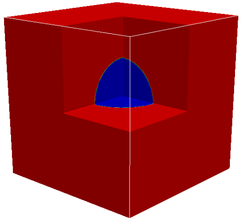


Figure 3: Spherical inclusion

A residual of 10^{-2} with a cost of $4000\ W_U$

W_U is the cost of one relaxation

CT Simulations

Mesh	Memory	Convergence	Property Jumps	Memory and Time
Voxel/ node	MF-FEM	?	?	?

	Single level	FMG scheme
Residual achieved	1.55×10^{-2}	7.89×10^{-6}
Cost / W_U	4139	19.6

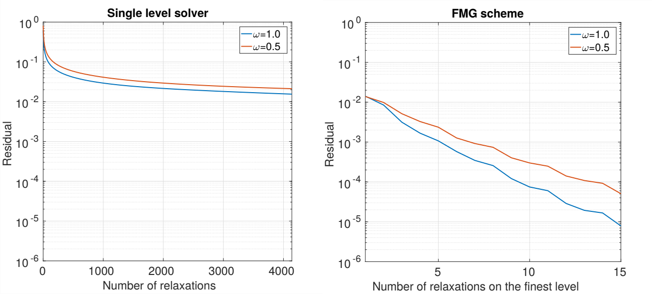
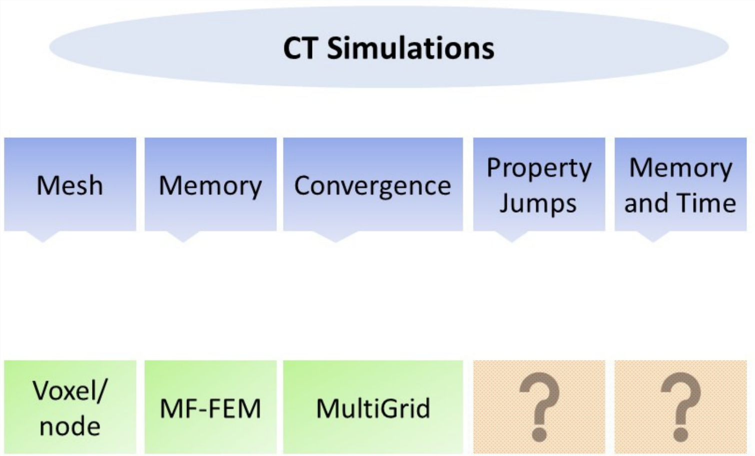
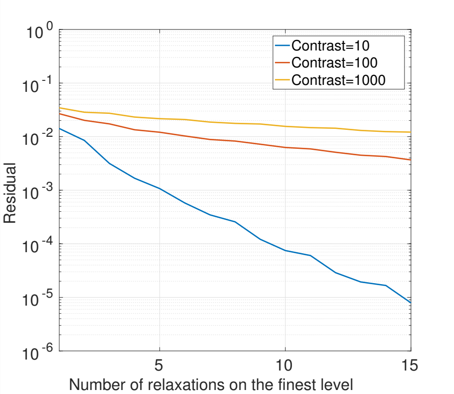


Figure 4: Convergence of single level (left) and FMG scheme (right) on a 129^3 nodes spherical thermal conduction problem with a contrast of 10

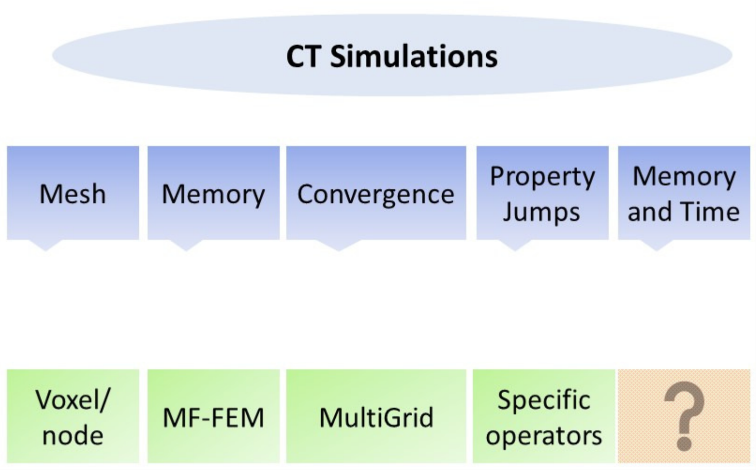

CT Simulations
Mesh
Memory
Convergence
Property Jumps
Memory and Time
Voxel/ node
MF-FEM
MultiGrid
?
?

MG convergence for high contrast

Convergence of MG on a 129^3 nodes spherical thermal conduction problem with different material property contrasts



Standard MG can **not** deal with problems with large variations


CT Simulations
Mesh
Memory
Convergence
Property Jumps
Memory and Time
Voxel/ node
MF-FEM
MultiGrid
Specific operators
?

- **memory** and **computational time**
- $2049 \times 2049 \times 2049$ voxels $\rightarrow$ more than 8×10^9 nodes
- 8 billion DoF $\rightarrow$ **239** days .
- 3×8 billion DoF $\rightarrow$ 3×**239** days $\approx$ **2 years** !!!.

Parallel computing must be implemented to avoid these difficulties

The solver has to be designed with a good parallel performance
Jacobi is a good candidate !

Supercomputer architecture

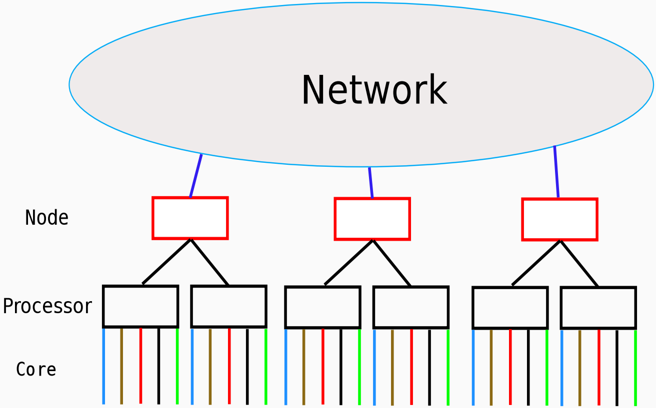
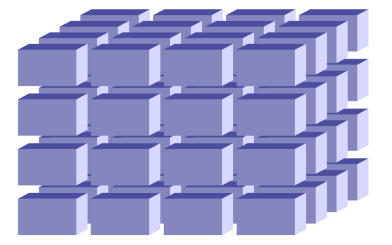


Figure 5: Architecture of Liger in ICI, Centrale Nantes

- Distributed memory: Message Passing Interface (MPI) **on** nodes
- Shared memory: OpenMP **in** node



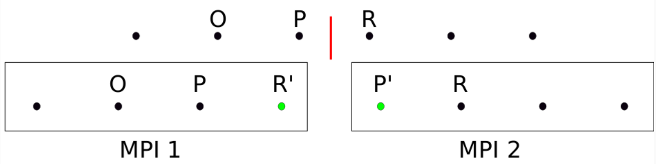


Figure 6: Ghost points

Coarsest grid: $4 \times 4 \times 4$ elements, i.e. no more than 64 MPI for this level

Hybrid MPI/OpenMP: several OpenMP / MPI

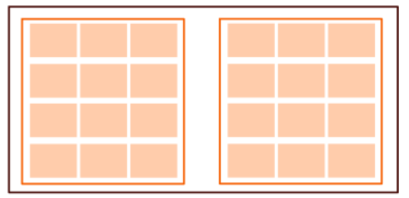


Figure 7: One node with 2 processors in Liger

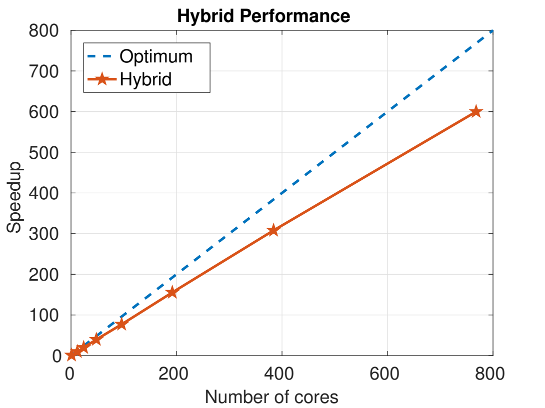
64 MPI × 12 OpenMP = 768 cores (Limited at 1 000 cores for each laboratory)

Advantages of Hybrid MPI/OpenMP:

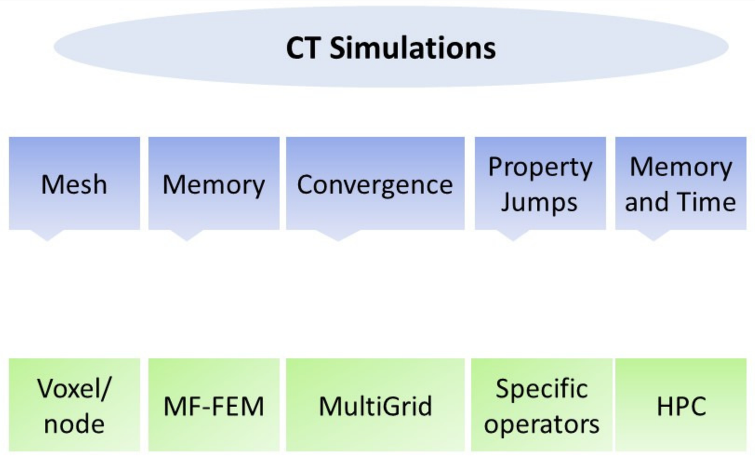
- Smaller memory requirement (fewer ghost points)
- Easier post processing (1 Output file / MPI)
- Suited for MG methods

Parallel performance

The figure is obtained by solving a one billion DoF problem.



768 cores: about 80% of optimum speedup.


CT Simulations
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MF-FEM
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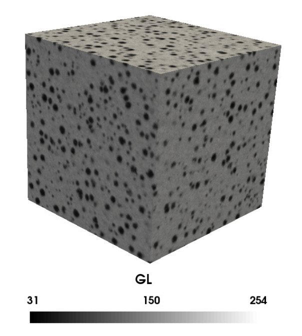
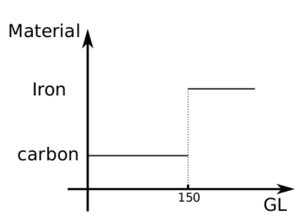
Specific operators
HPC

Nodular graphite cast iron image

Image obtained by RANNOU *et al.*
Region Of Interest (ROI): $257 \times 257 \times 257$ voxels, $\approx$50 million DoF

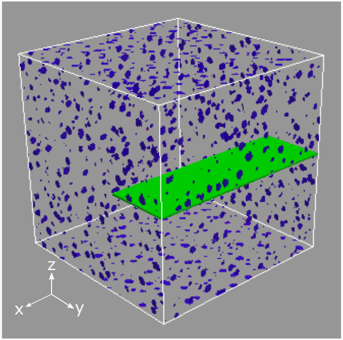




where *GL* is the gray level on each voxel, which is an integer between 0 and 255.

RANNOU J., LIMODIN N., RÉTHORÉ J., GRAVOUIL A., LUDWIG W., BAÏETTO -DUBOURG M.-C., BUFFIERE J.-Y., COMBESCURE A., HILD F., ROUX S., Computer methods in applied mechanics and engineering, 199, 1307-1325, 2010.

- Iron: $E = 210$ GPa, ν= 0.3
- Carbon: $E = 21$ GPa, ν= 0.2
- Size: L×L×L
- Crack thickness: 3 voxels
- $Strain_o = 1\%$



Boundary conditions:

$$\begin{cases} u_z = 0, & \text{on } Z = -\frac{L}{2} \\ u_z = 0.01L, & \text{on } Z = \frac{L}{2} \\ \vec{\hat{u}} = \vec{0}, & \text{at } (0,0,-\frac{L}{2}) \end{cases}$$

Crack opening

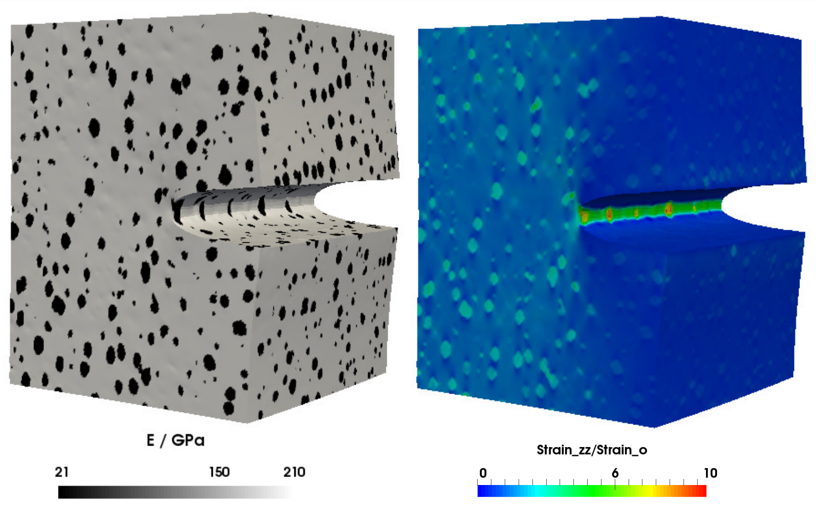


Figure 8: The Young's modulus and the strain$_{zz}$ in cast iron. The displacement is multiplied by a factor of 20.

Crack opening

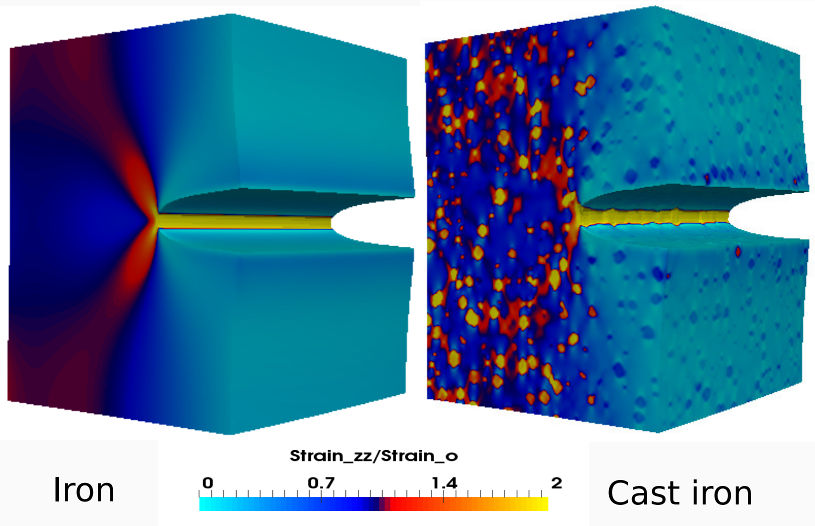


Figure 9: $Strain_{zz}$ in iron and in cast iron. The displacement is multiplied by a factor of 20.

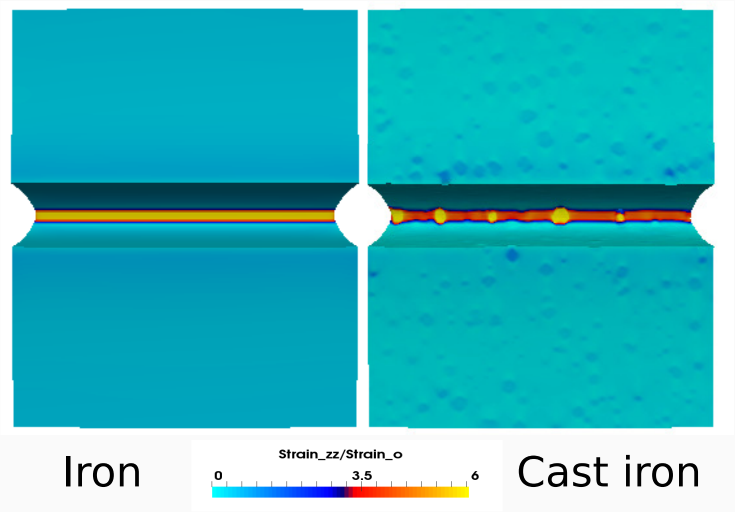
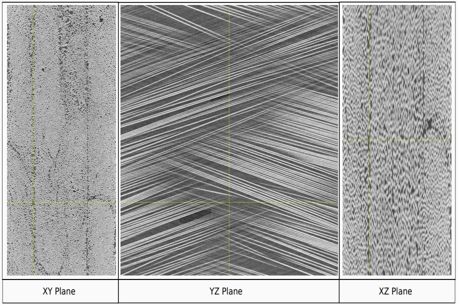


Figure 10: Strain concentrations on the crack font in the cast iron and in the iron. The displacement is multiplied by a factor of 20.

Laminate composite material

The image of a composite material obtained by Lecomte-Grosbras et al.(2015): E-glass fiber with M9 epoxy resin

- $700 \times 1700 \times 1300$ voxels
- Four layers: $15°$, $-15°$, $-15°$ and $15°$



Lecomte-Grosbras, P., Réthoré, J., Limodin, N., Witz, J.-F., Brieu, M., 2015. Three-dimensional investigation of free-edge effects in laminate composites using x-ray tomography and digital volume correlation. Experimental Mechanics 55 (1), 301–311.

Experimental results obtained by digital image correlation (DIC)

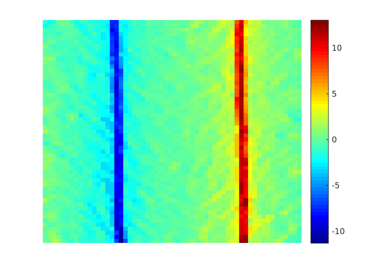
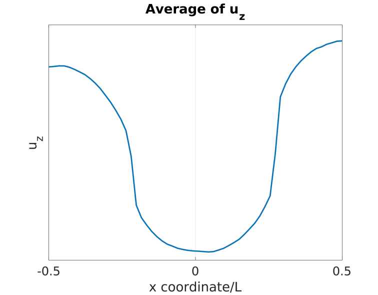


Figure 11: Stain_{xz}

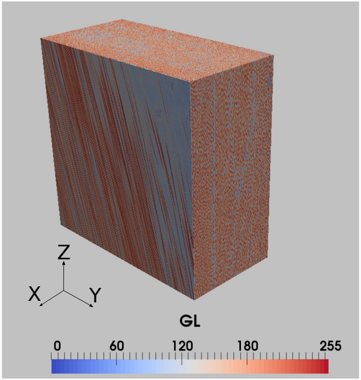


Free edge effects in this laminate structure

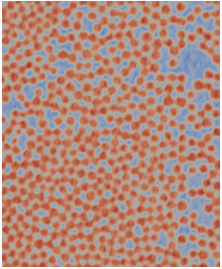
- Strain concentrations in the ply interface
- Large displacement gradient in the ply interface

Lecomte-Grosbras, P., Réthoré, J., Limodin, N., Witz, J.-F., Brieu, M., 2015. Three-dimensional investigation of free-edge effects in laminate composites using x-ray tomography and digital volume correlation. Experimental Mechanics 55 (1), 301–311.

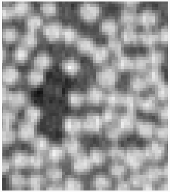
3D image

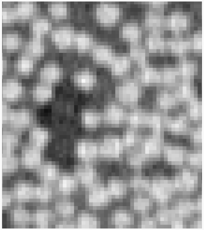


Zoom



Zoom Zoom





Trial and error method

$$\alpha = \left(1 - e^{-\frac{|GL-160.5|}{20}}\right) \cdot sign\,(GL - 160.5) + 1$$

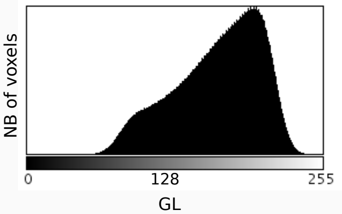
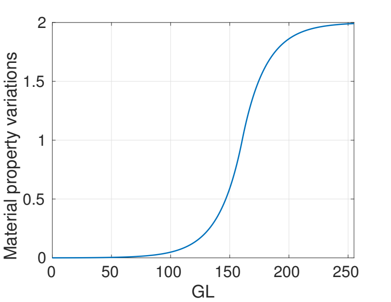


Figure 12: Histogram



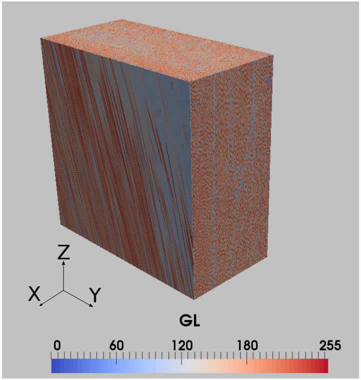
Material property

ROI: $577 \times 1153 \times 1153$, *i.e.* about 0.8 billion voxels

- E-glass fiber: $E = 80.0$ GPa, $\nu = 0.22$
- Epoxy: $E = 3.2$ GPa, $\nu = 0.22$

Subsampling into
$1153 \times 2305 \times 2305$ voxels
$\approx$6 billion voxels or 18 billion DoF.
Size: L×2L×2L
$Strain_o = 1\%$

$$\begin{cases} \vec{u} = \{0,\ 0,\ -0.01L\}, & \text{on } z = -L \\ \vec{u} = \{0,\ 0,\ 0.01L\}, & \text{on } z = L \end{cases}$$



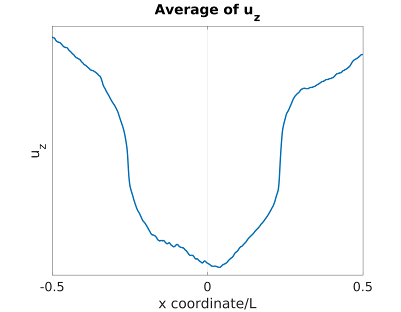


Figure 13: Numerical results

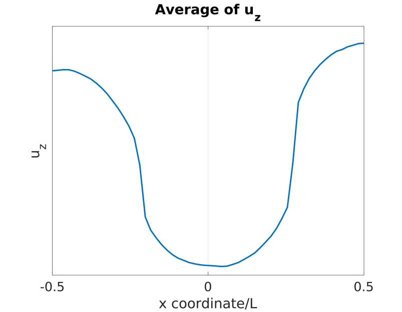
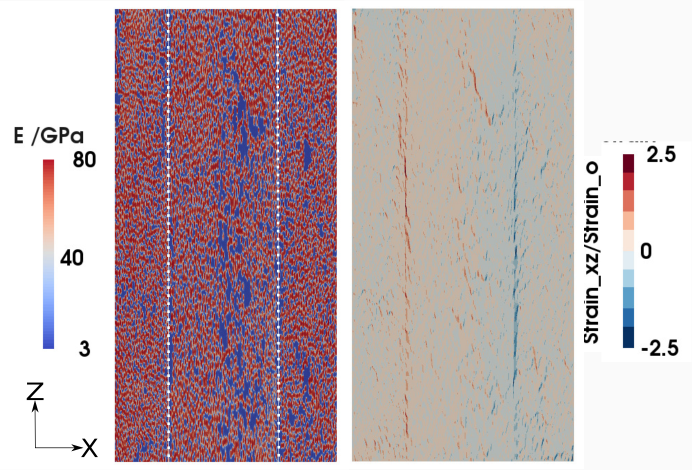


Figure 14: Experimental results

A good correlation can be found between the numerical simulation and the DIC experiment.

LECOMTE-GROSBRAS P., PALUCH B., BRIEU M., D E S AXC É G., SABATIER L., Composites Part A: Applied Science and Manufacturing, 40, 1911-1920, 2009.

Numerical result



Strain concentrations in ply interface.

Numerical result

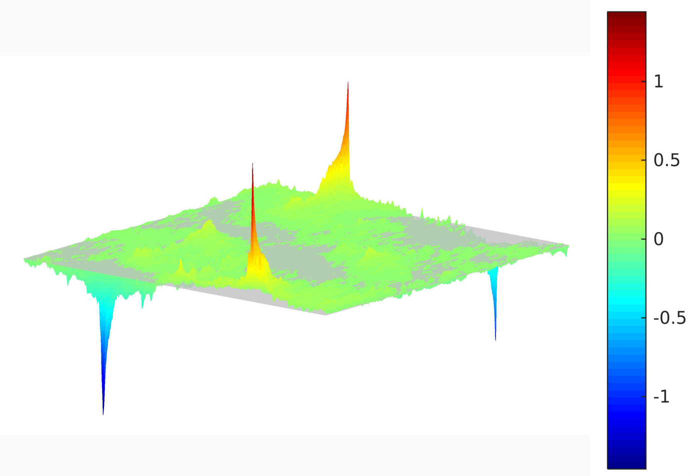


Figure 15: Averages of $Strain_{xz}/Strain_o$ along axis Z

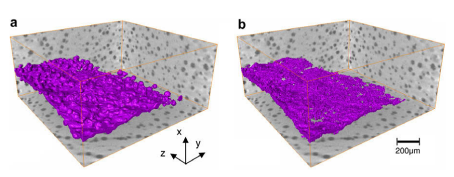
Conclusions

- The simulation with a large real tomography image (18 billion DoF) is performed
- The proposed strategy permits to analyze deformation mechanism at the microscopic scale
- The qualitative agreement between the simulation and the DIC experiment confirms the accuracy to perform CT simulations
- The interaction between the crack and the microstructure shows the indispensability to perform CT simulations

X. liu, J. Réthoré, M.-C. Baietto, P. Sainsot, A.-A.. Lubrecht, An efficient strategy for large scale 3D simulation of heterogeneous materials to predict effective thermal conductivity, Computational materials science, 166, 265–275, 2019.
X. liu, J. Réthoré, M.-C. Baietto, P. Sainsot, A.-A.. Lubrecht, A massively parallel matrix free finite element based multigrid method for simulations of the mechanical behavior of heterogeneous materials using large scale CT images, Computational Mechanics, online.
IDS ConnectTalent project funded by Région Pays de la Loire and Nantes Métropole

Perspectives

- A quantitative comparison between the simulation and the DIC experiment is advised
  - Apply the measured boundary conditions
  - Identify real material property of each constitutive
- Phase field method to compute the crack propagation



- Up-scaling mechanical fields to incorporate crack / μstructure interaction in a macroscale model. Elie EID PhD thesis, ANR JCJC METACRACK project.

A massively parallel matrix free FE-based multigrid method for simulating the behavior of heterogeneous materials using large scale CT images

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