An efficient strategy for phase field modeling of fracture in heterogeneous materials from 3D images

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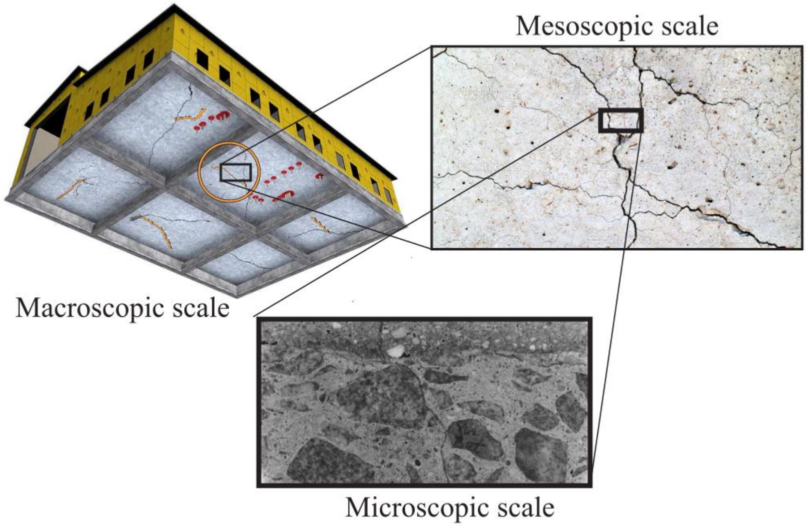
Background

- Plenty of engineering accidents and problems are due to fractures



- Fractures usually start by micro-cracks

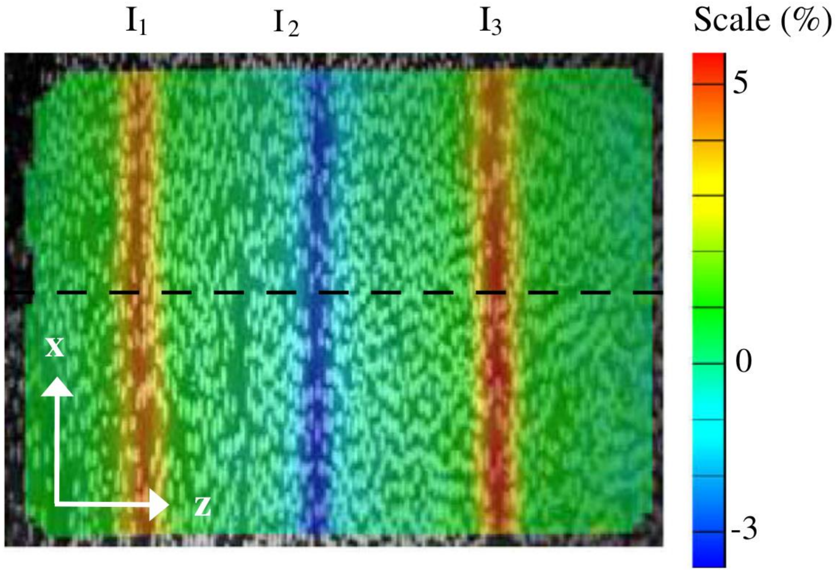
Thanh, Tung, NGUYEN, Ph.D Thesis, 11, 2015

Background

Macro-structure, i.e. **homogenized** structure, loses **local details**

e.g. free-edge effects in laminated composite materials

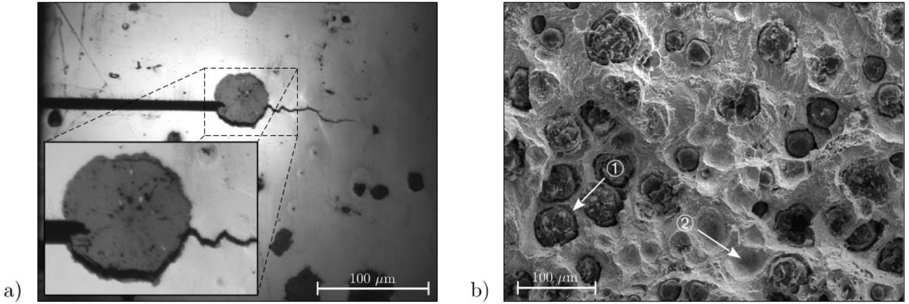
Real µ-structures using CT images



P., Lecomte-Grosbras et. al., Composites: Part A, 2009.

Challenges and Objective

- **Real** 3D images of **heterogeneous** materials
- **Complex** µ-structures
- **Large** material properties jumps
- **Huge** computational cost both on time and memory



An **automatic** and **efficient** solver without any idealizations

J., LACHAMBRE, Ph.D Thesis, 05, 2014.

Numerical model

Staggered phase field

- Loop on time step t
  - Compute displacement
  - Calculate strain history
  - Calculate phase field
- end loop

$$\begin{cases} d = 0 & \Psi^+ < \Psi^- \\ \nabla \cdot \boldsymbol{\sigma} = \boldsymbol{0} & \text{in } \Omega \\ \boldsymbol{u} = \boldsymbol{U}_0 & \text{on } \partial\Omega_D \\ \boldsymbol{\sigma} \cdot \boldsymbol{n} = \boldsymbol{f}_{ext} & \text{on } \partial\Omega_N \end{cases}$$

$$\mathcal{H}(\vec{x}, t) = max(\Psi^+(\epsilon(\vec{x}, t)))$$

$$\begin{cases} 2(1-d)\mathcal{H} - \frac{g_c}{\ell_c}(d - l^2 \Delta d) = 0 & \text{in } \Omega \\ d(\boldsymbol{x}) = 1 & \text{on } \Gamma \\ \nabla d(\boldsymbol{x}) \cdot \boldsymbol{n} = 0 & \text{on } \partial\Omega \end{cases}$$

Expensive: Thousands of time steps

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Real image-based Simulations

Mesh	Memory	Convergence	Property Jumps	Time
?	?	?	?	?

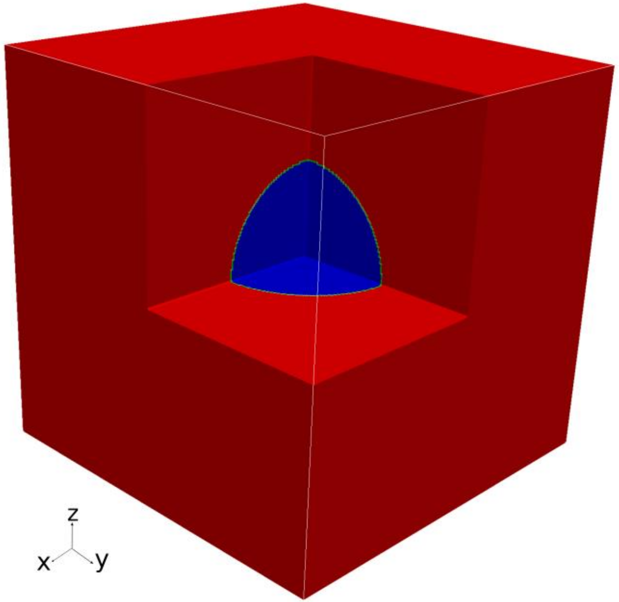
Numerical methods

- **Finite element methods with 1 voxel / node**
  - Automatic mesh generation
- **Matrix-free method**
  - Reduced memory requirement, *e.g.* **81** times **cheaper** than the global sparse stiffness matrix for a 3D mechanical problem
- **Preconditioned conjugate gradient (PCG) solver**
  - Handle large variations
  - Avoid FEM lock effects, i.e. large Poisson coefficient
- **Geometric MultiGrid (MG) accelerator**
  - fine grid: eliminate high-frequency error
  - coarse grid: eliminate low-frequency error

Performance analysis

Spherical inclusion for a linear elastic problem

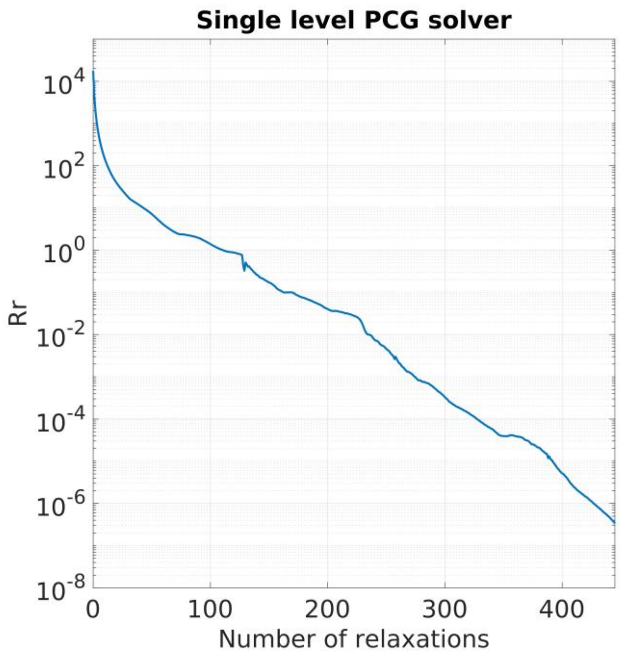
- Nb of elements: 128^3, i.e. 2 million
- Traction along Z
- E_M = 233.43 GPa
- E_i = E_M / 1000
- ν=0.29



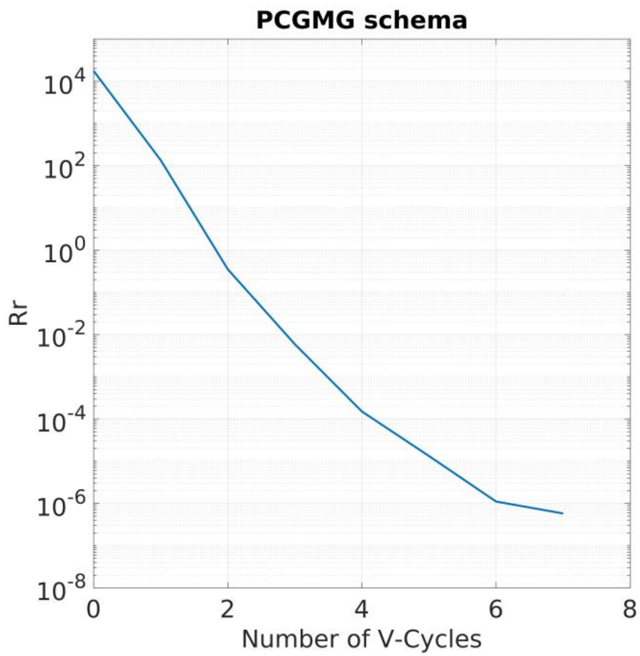
Relative residual :

$$Rr = \frac{\vec{r}^T \cdot \vec{r}}{\vec{F}_R^T \cdot \vec{F}_R}$$

Performance analysis



445 relaxations



≈17 relaxations

Multilevel PCG is **26** times **cheaper**

Real image-based Simulations

Mesh	Memory	Convergence	Property Jumps	Time
Voxel/ node	Matrix free	MultiGrid	?	?

Complex jumps

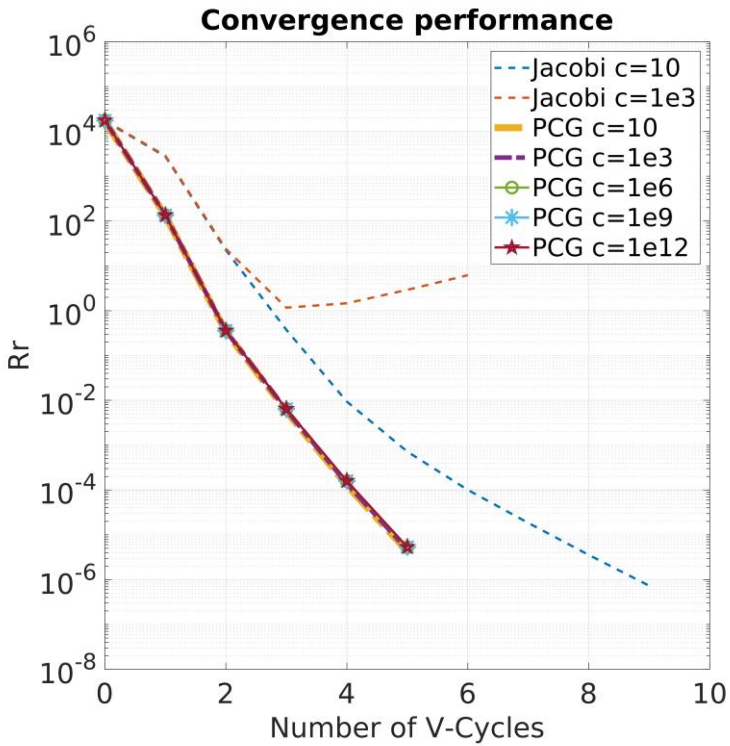
Robust

- huge contrast, *e.g.* 10^{12}

***Limitations** of the spherical inclusion :*

- *Simple geometry*
- *Mano inclusion*
- *Theoretical image*

Real images?

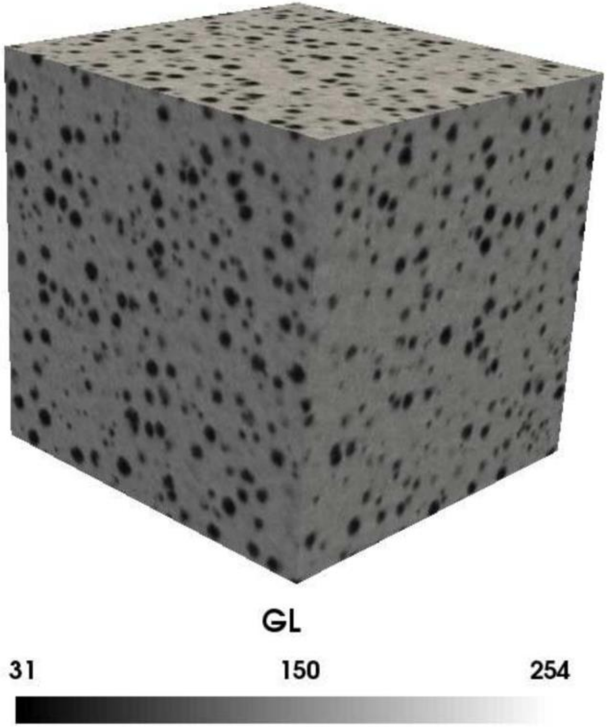


Complex jumps

Linear elastic problem with stress singularity

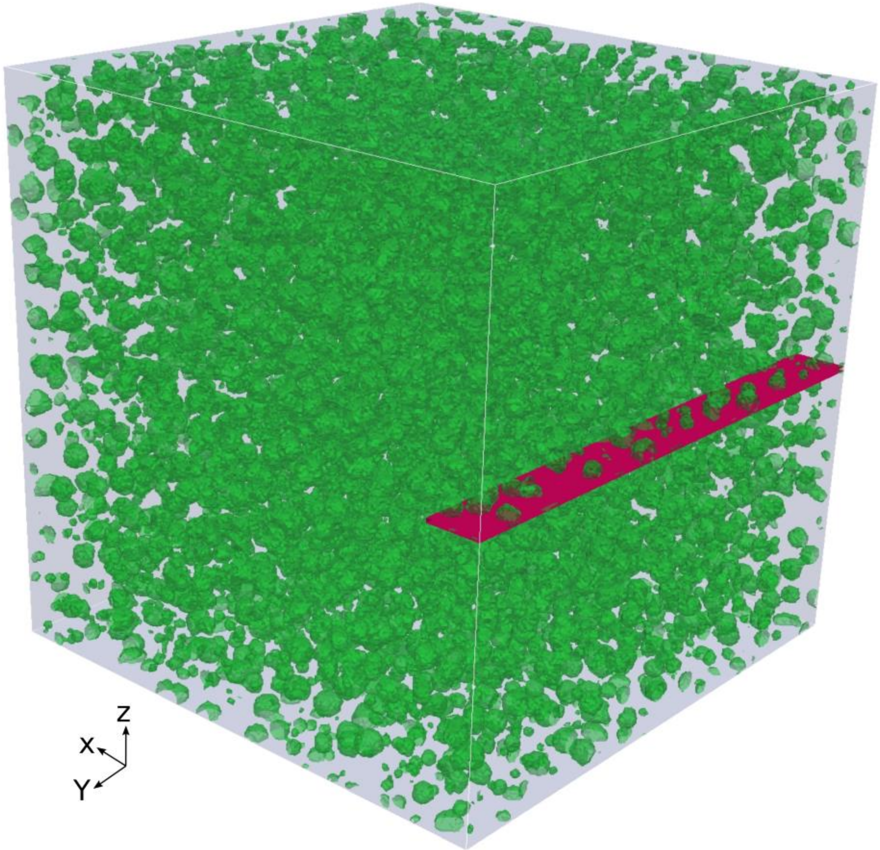
- ROI taken from image of graphite cast iron
- Nb of voxels: 256^3, *i.e.* 16 million

Material	E / GPa	ν	$g_c/J \cdot m^{-2}$
Iron	210	0.2	1730
Graphite nodules	21	0.3	180

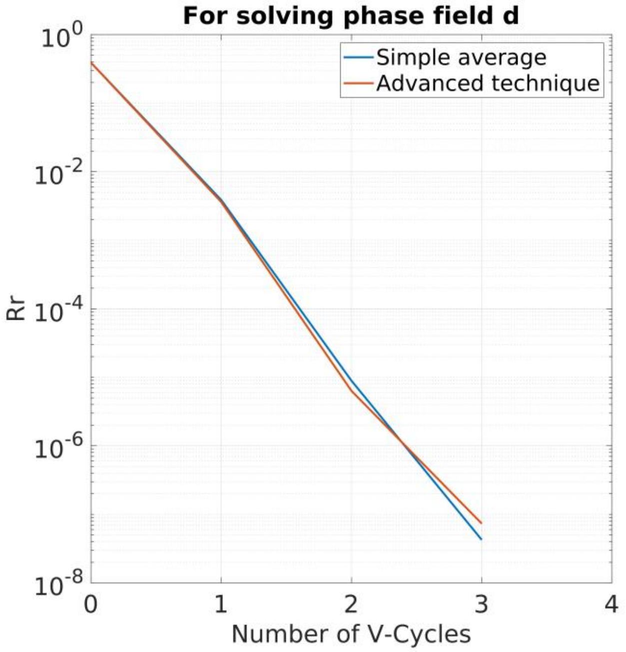


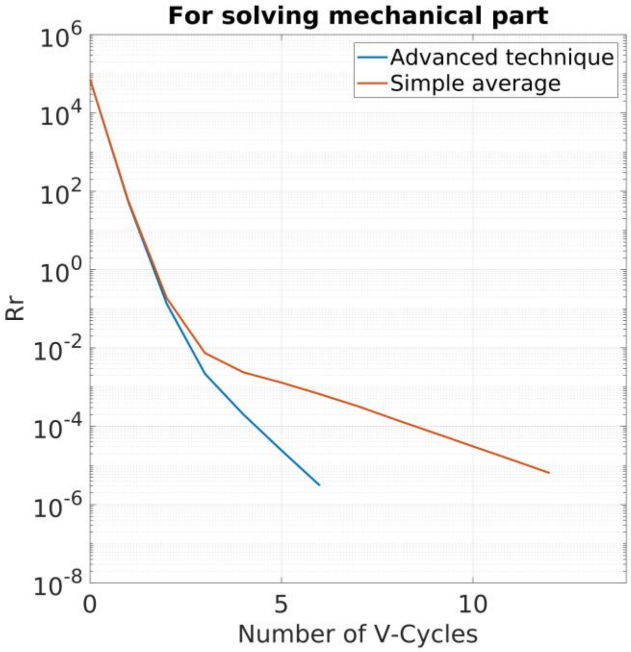
J., Rannou et. al., CMAME, 2010.

Complex jumps



Complex jumps





Advanced technique is **2** times **faster**

Real image-based Simulations

Mesh	Memory	Convergence	Property Jumps	Time
Voxel/ node	Matrix free	MultiGrid	Advanced technique	Hybrid MPI/OMP

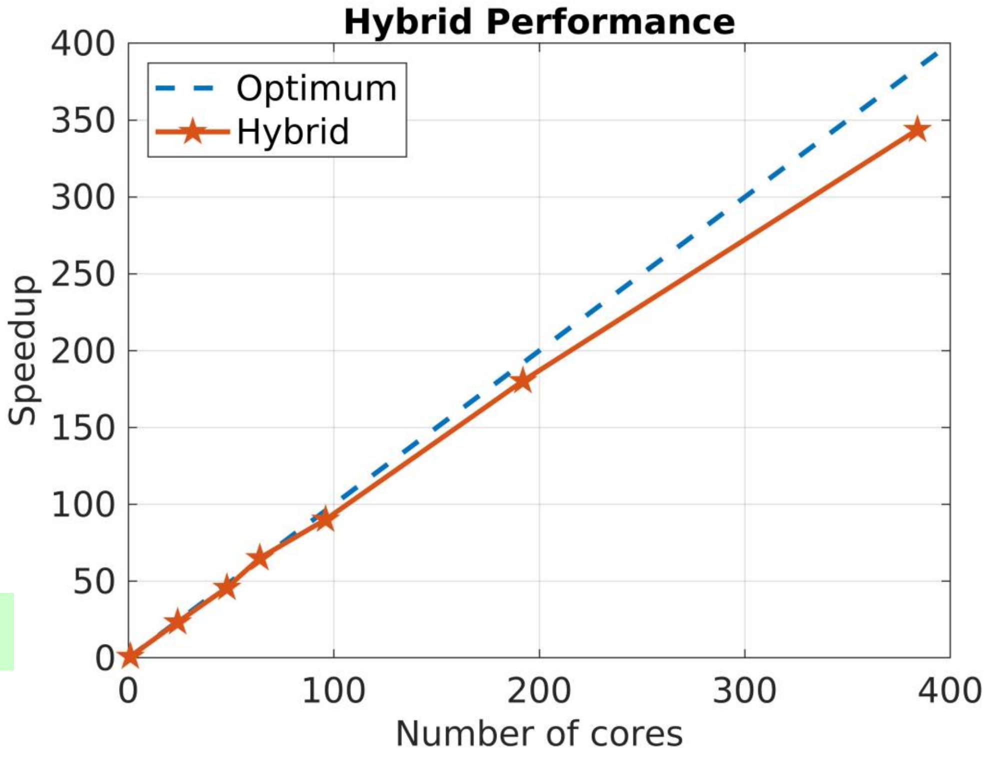
Parallel performance

Efficiency

90% for this problem with 16 million elements

400 cores

1 year → **1 day**

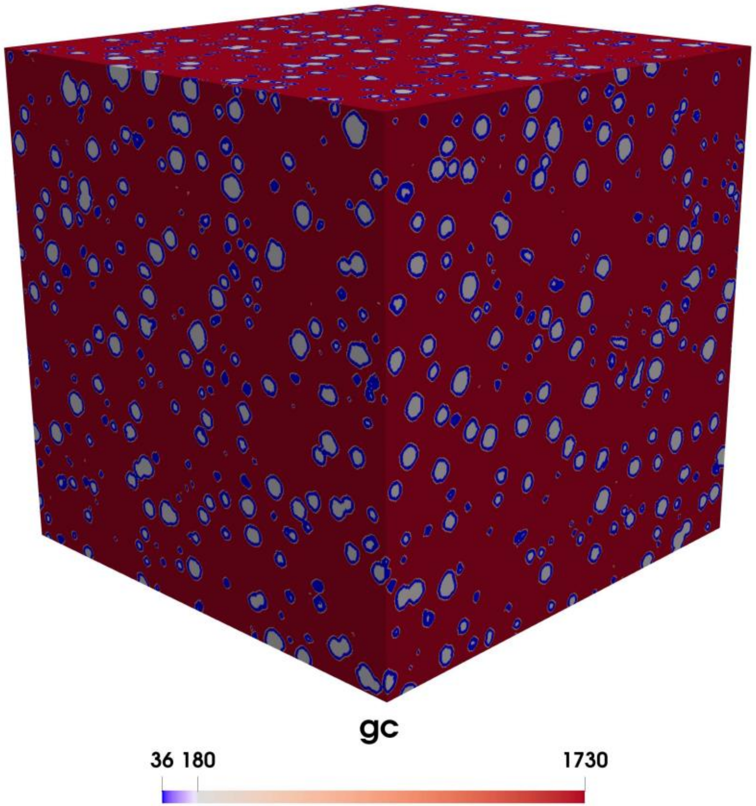


Applications

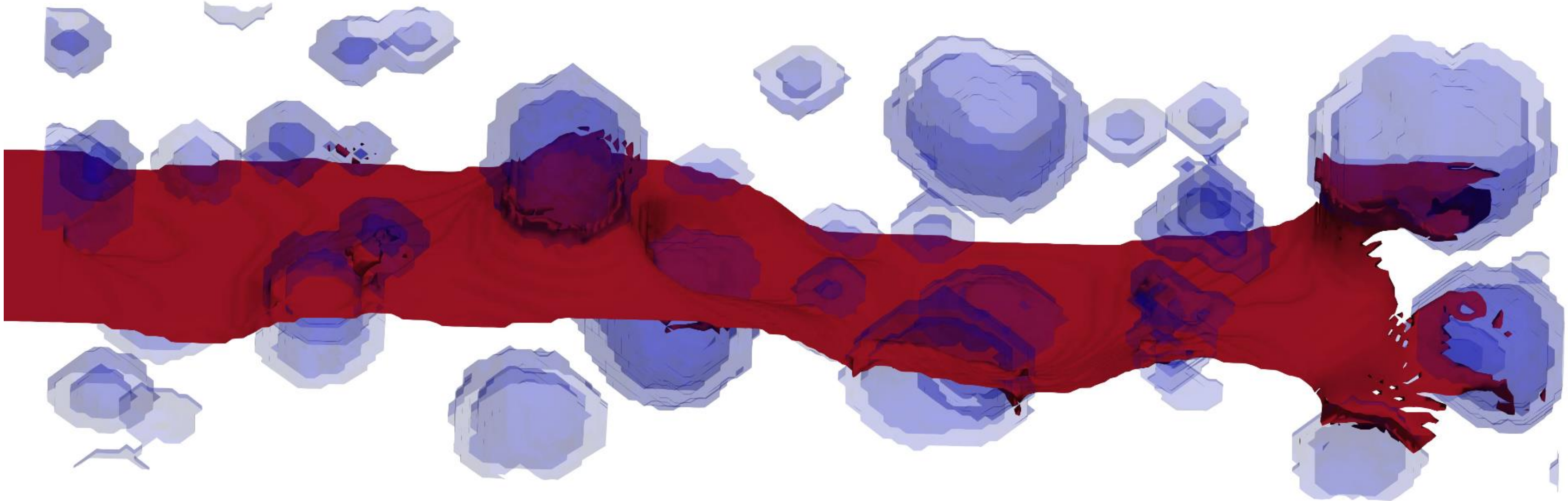
Crack propagation in graphite cast iron with a prescribed initial crack

- ROI + tri-linear interpolation
- Nb of voxels: 512^3, *i.e.* 134 million
- To have enough voxels in **interfaces**

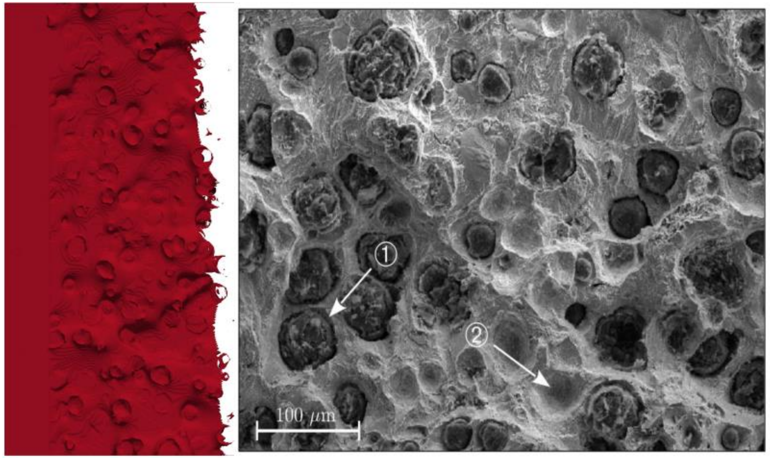
Material	E / GPa	ν	$g_c/J \cdot m^{-2}$
Iron	210	0.2	1730
Graphite nodules	21	0.3	180
Interface			**36**

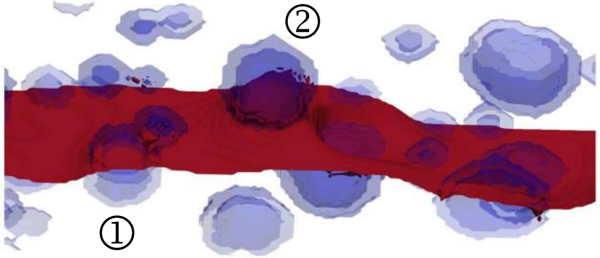


Crack propagation



Crack propagation





Experiment

- ① Anchor nodule
- ② Torn nodule

Simulation

Conclusions

- An **efficient** and **automatic** strategy for simulations of fractures
  - Simulations at the scale of voxel to avoid any idealizations (segmentations)
  - Efficient and robust PCG based MG algorithms
  - High parallel efficiency
- A strong macro-micro **interaction** is demonstrated
  - Crack path is affected by material properties
- A good experiment-simulation **agreement** is found

X., Liu et. al., CMAME, 2022.

Thank you!