Prediction of grain size evolution during thermal and thermomechanical treatments at the mesoscopic scale: numerical improvements and industrial examples

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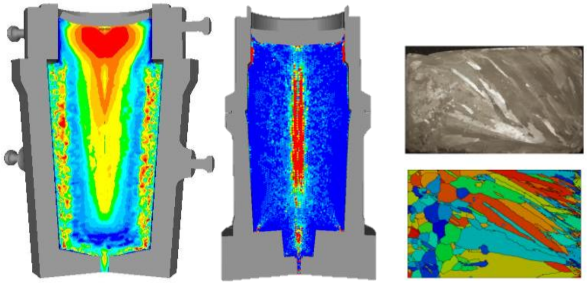
CONTEXT

- **A growing interest for microstructure modelling throughout the whole process chain…**

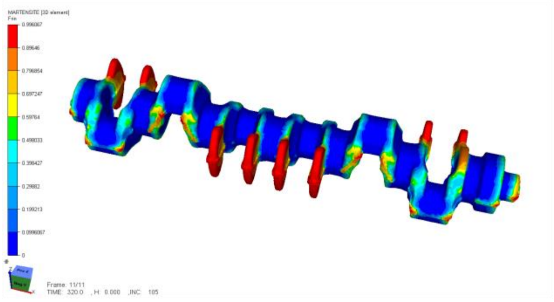
Solidification



Carbon segregation | Porosities | Grain structure

THERCAST®

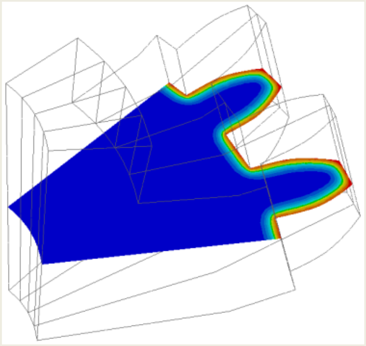
Heat treatments



Phase fractions

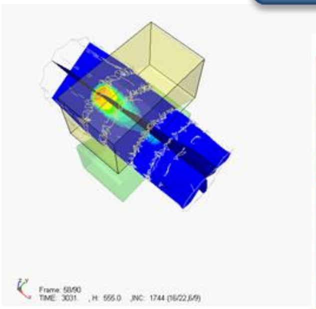
FORGE®

Thermochemical treatments

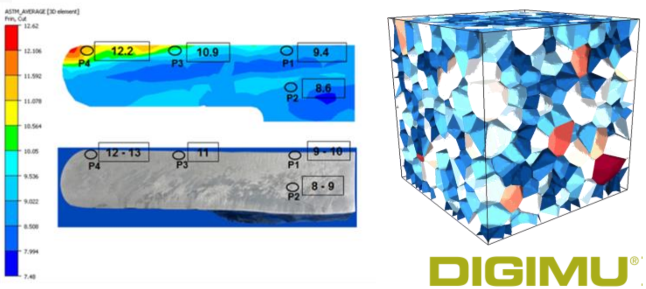


Chemical diffusion

Forming processes



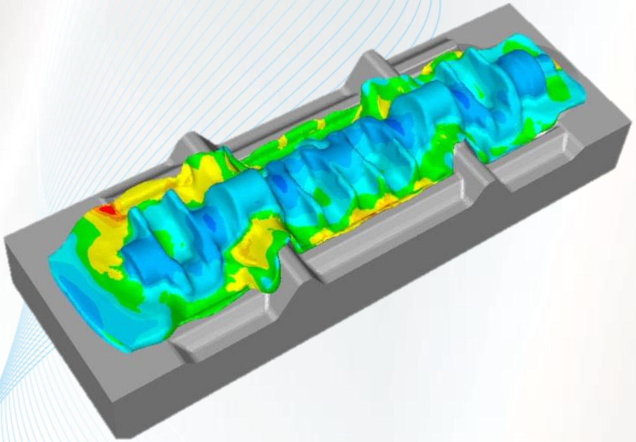
Porosities closure



Grain structure

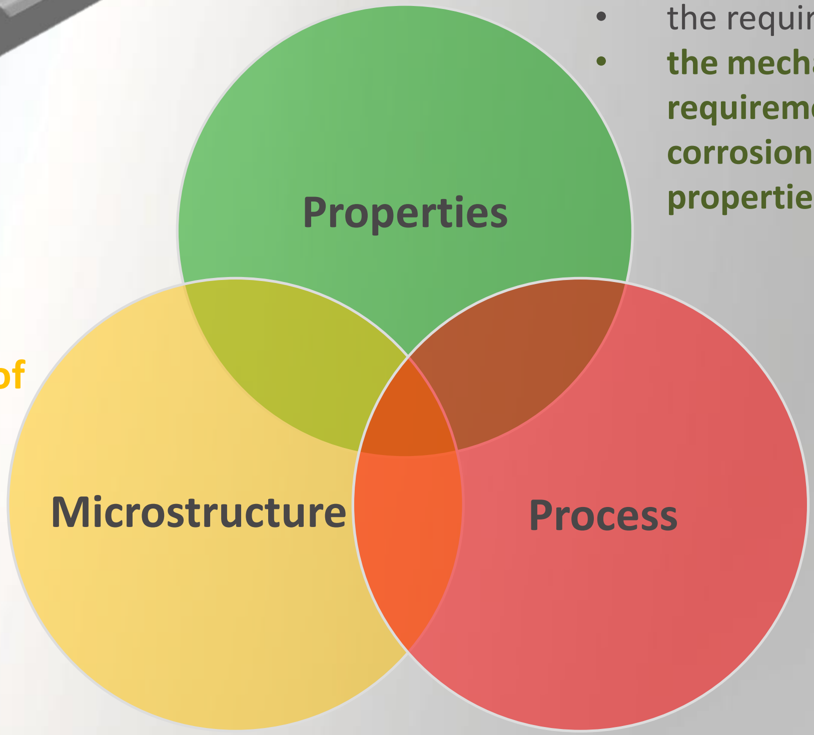
CONTEXT

- **… and particularly during hot forming processes**



For the parts made, hot forging scheme must ensure:

- the required shape and size
- **the mechanical performance requirements (strength, toughness, corrosion resistance, high-temperature properties…)**



Decisive effect of the grain size

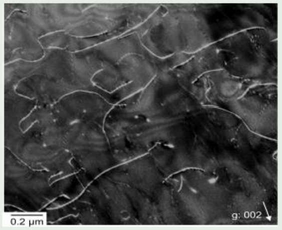
Adapted thermomechanical processing route

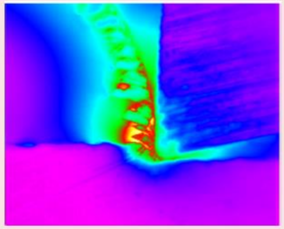
CONTEXT

Microstructural evolution

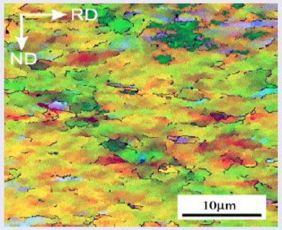
- Governed by the process parameters (temperature, strain and strain rate)
- Given by reduction of the internal energy

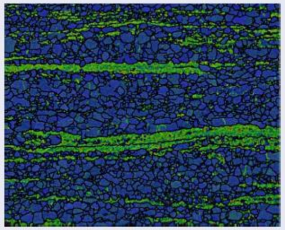

Deformation

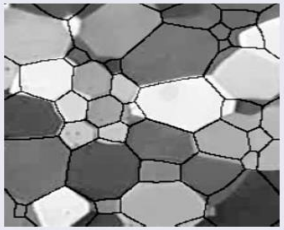

Stored energy


Heat

The way to return to equilibrium


Recovery

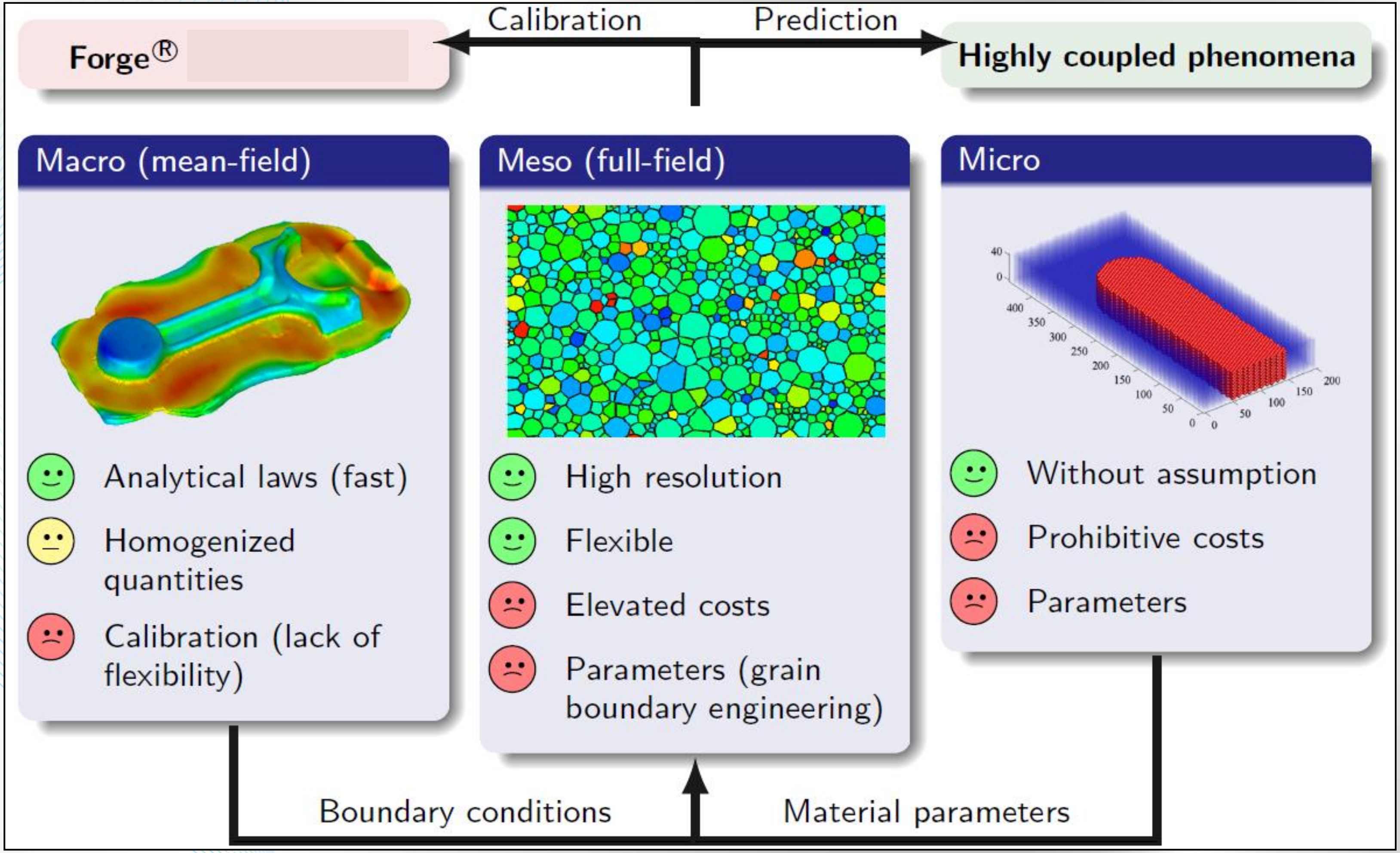

Recrystallization


Grain growth

Necessity to model the different metallurgical phenomena to predict the microstructural evolution

CONTEXT

- **Modelling scales**



Calibration → Forge® | Prediction → **Highly coupled phenomena**

Macro (mean-field)

- 🙂 Analytical laws (fast)
- 😐 Homogenized quantities
- 🙁 Calibration (lack of flexibility)

Meso (full-field)

- 🙂 High resolution
- 🙂 Flexible
- 🙁 Elevated costs
- 🙁 Parameters (grain boundary engineering)

Micro

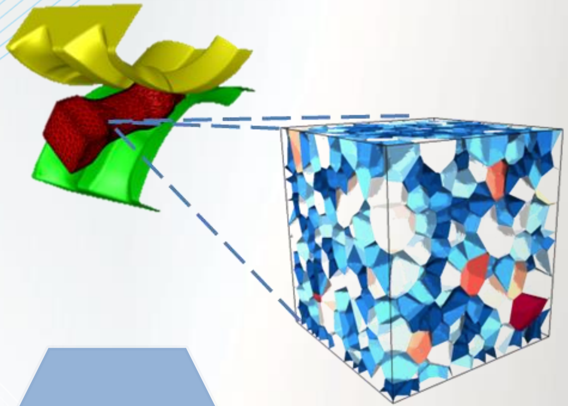
- 🙂 Without assumption
- 🙁 Prohibitive costs
- 🙁 Parameters

Boundary conditions → Meso ← Material parameters

CONTEXT

Mesoscale modelling – Full field approach

- Modelling the evolution of the grains (microstructure components fully modelled)
- Simulations performed on Representative Volume Elements (RVE)



Different model categories

- Vertex
- Phase field
- Monte Carlo
- Cellular Automaton
- **Level Set**

+ **Realistic description of microstructural features**
  - Topological aspects taken into account
  - Help for understanding microstructural phenomena
  - Modelling local and heterogeneous phenomena

+ **Concept of numerical tests (scale transition)**
  - Improvement of higher scale models usable for macroscopic simulations
  - Calibration of these models

− **Computation time**
  - Simulation performed on specific locations of an industrial workpiece (thermomechanical and thermal history as boundary conditions applied to the RVE)

OUTLINE

- Context

- Mesoscale modelling in a Level-Set framework
  - DIGIMU®: mesoscale computations in an industrial context
  - Generation of polycrystals in a finite element context
  - Grain boundary migration modelling
  - Numerical improvements

- Application examples
  - Pure grain growth
    - Solutionizing in one-phase field
    - HIP bonding
  - Presence of second phase particles
    - Smith-Zener pinning phenomenon
    - Control of the grain size in an ODS steel
    - Understanding of the abnormal grain growth phenomenon
  - Hot forming processes

- Conclusion

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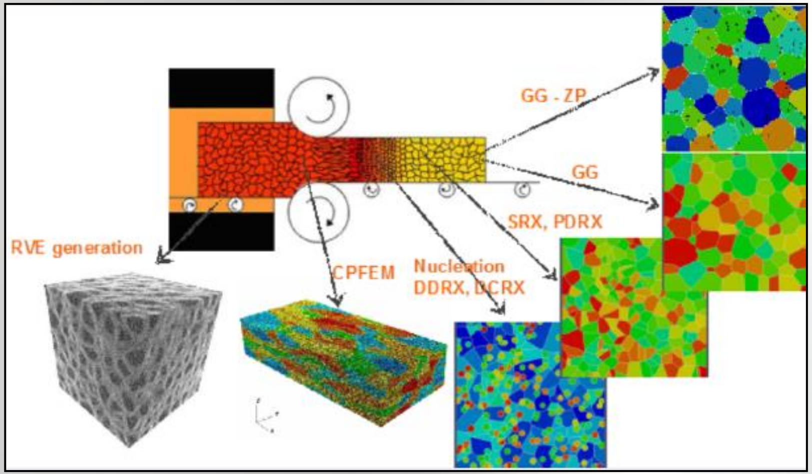
DIGIMU®: MESOSCALE COMPUTATIONS IN AN INDUSTRIAL CONTEXT

- **From simulations for industry towards simulations by industry**

Development of an industrial solution for simulating microstructural evolutions at the grains scale during thermomechanical processes



Our industrial partners

Digimu - ANR Industrial Chair (2016-2020)

Chaire ANR ARCELORMITTAL AREVA ASCOMETAL AUBERT&DUVAL CEA SAFRAN TRANSVALOR

GENERATION OF POLYCRYSTALS IN A FE CONTEXT

Microstructure immersion in a FE mesh

Implicit description of the interfaces using a level-set framework

- What is a level-set function?

Signed distance function

$$\begin{cases} \psi(x,t) = \pm d(x,\Gamma(t)), \ x \in \Omega \\ \Gamma(t) = \{x \in \Omega, \psi(x,t) = 0\} \end{cases}$$

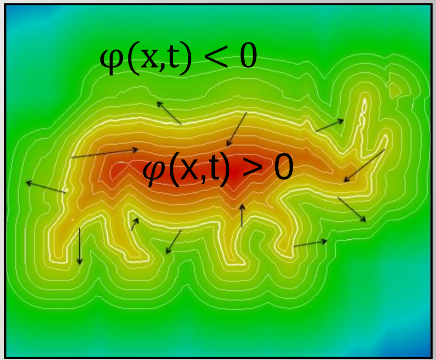
- Evolving interfaces

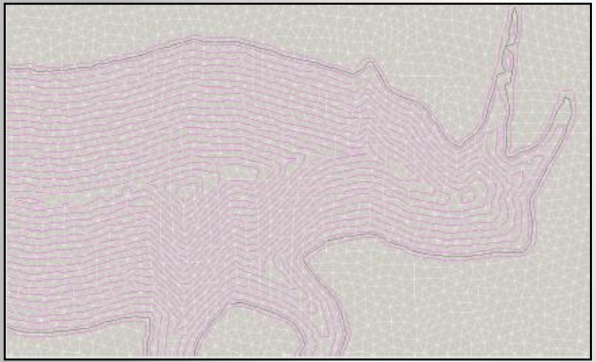
Transport of a LS function

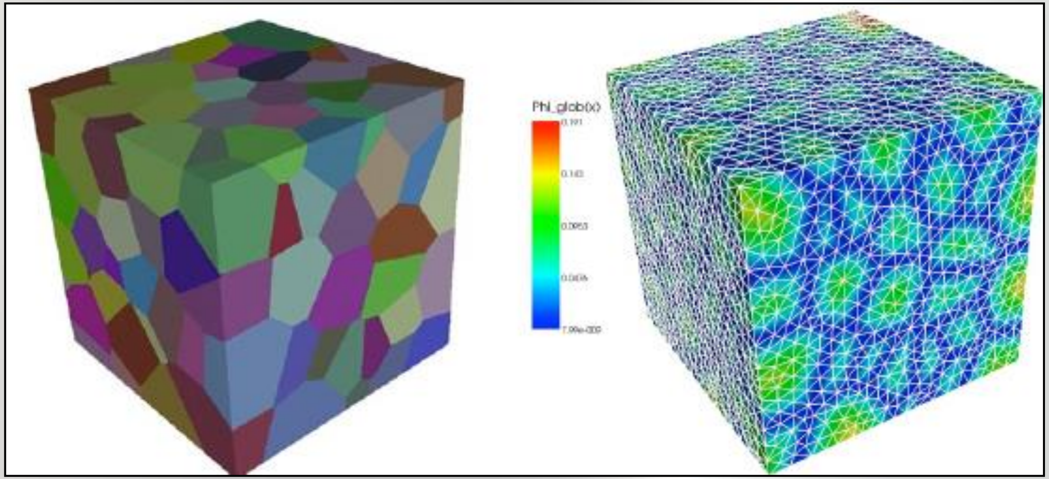
$$\begin{cases} \dfrac{\partial \psi(x,t)}{\partial t} + \vec{v} \cdot \nabla \psi = 0 \\ \psi(x, t=0) = \psi^0(x) \end{cases}$$

- Immersion of a polycrystal into a FE mesh
  - ○ Statistical random processes (Laguerre Voronoï tesselation)
  - ○ Experimental images

➔ Extension to several LS functions







[Bernacki et al., 2008], [Bernacki et al., 2009], [Bernacki et al., 2011], [Fabiano et al. 2014], [Hitti et al. 2012]

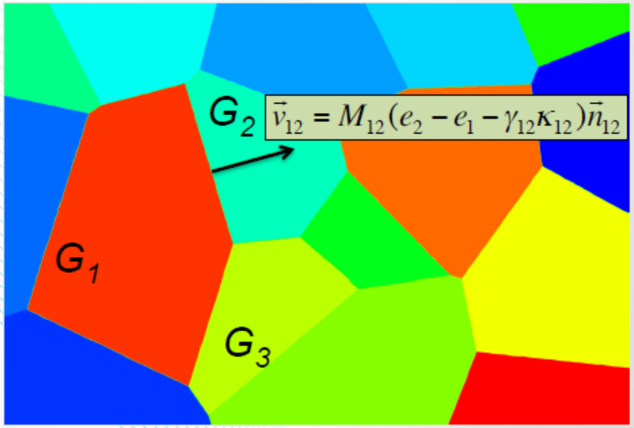
GRAIN BOUNDARY MIGRATION MODELLING

Normal velocity of a grain boundary

$$\vec{v} = m\boxed{(\tau\Delta\rho - \gamma\kappa)}\,\vec{n} \qquad \left\{\begin{array}{l} m : \text{grain boundary mobility} \\ \gamma : \text{grain boundary energy} \\ \kappa : \text{grain boundary mean curvature} \\ \tau\Delta\rho : \text{stored energy} \\ \vec{n} : \text{outward normal unit vector} \end{array}\right.$$

Thermodependent

Driving force for grain boundaries motion



- Convective-diffusive approach

$$\left\{\begin{array}{ll} \dfrac{\partial\psi_i(x,t)}{\partial t} - M\gamma\Delta\psi_i(x,t) + \vec{v}_e\cdot\nabla\psi_i(x,t) = 0, & \forall i \in \{1,\ldots,N_p\} \\ \psi_i(x,t=0) = \psi_i^0(x), & \end{array}\right.$$

$$\vec{v}_e(x) = M\sum_{i=1}^{N_p}\sum_{\substack{j=1\\ j\neq i}}^{N_p}\chi_i(x) f\left(\psi_j(x),l\right)\left(\mathcal{E}_i(x) - \mathcal{E}_j(x)\right)\frac{\nabla\psi_j(x)}{\|\nabla\psi_j(x)\|}$$

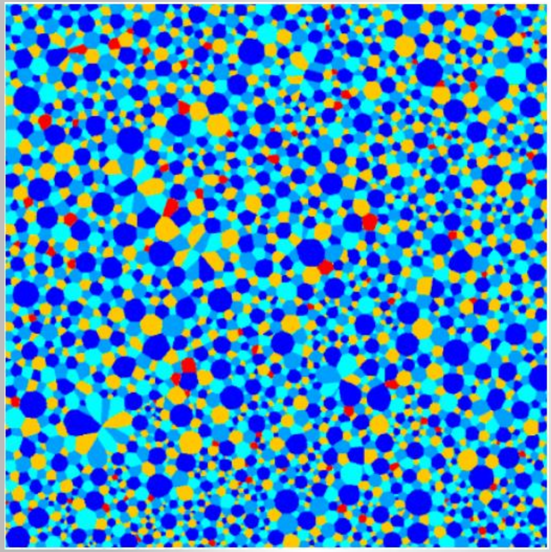
NUMERICAL IMPROVEMENTS

- **How to reduce computation times?**

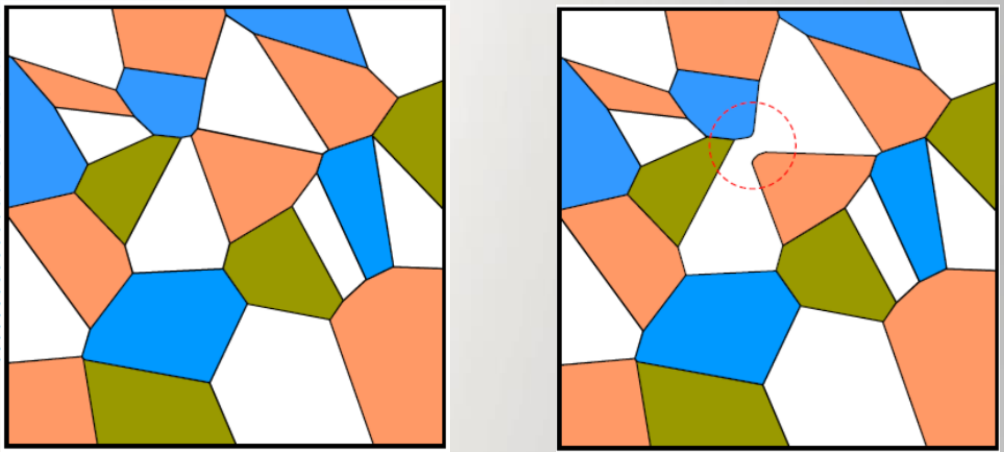
Reduce the number of LS functions

- Use of *Global Level Set functions*: a set of initially distinct grains can be packed in a single LS function

- Associated with evolutive graph coloring technique to avoid numerical coalescence : *Swapping algorithm*



Microstructure composed of 3680 grains represented by 5 GLS functions



25 grains represented by 4 colors

Coalescence

[Scholtes et al. 2015]
[Scholtes et al. 2016a]

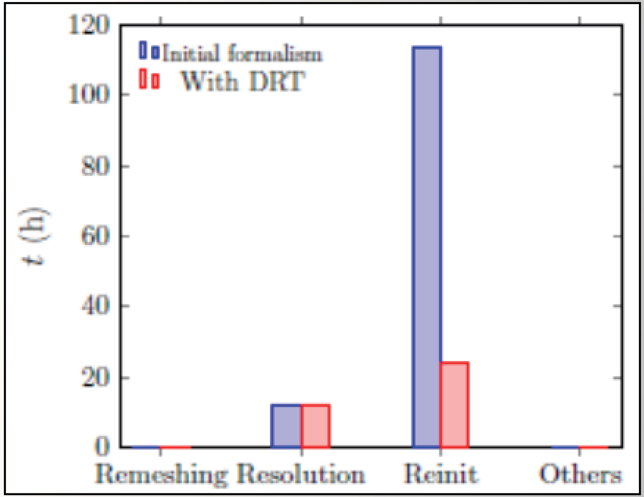
NUMERICAL IMPROVEMENTS

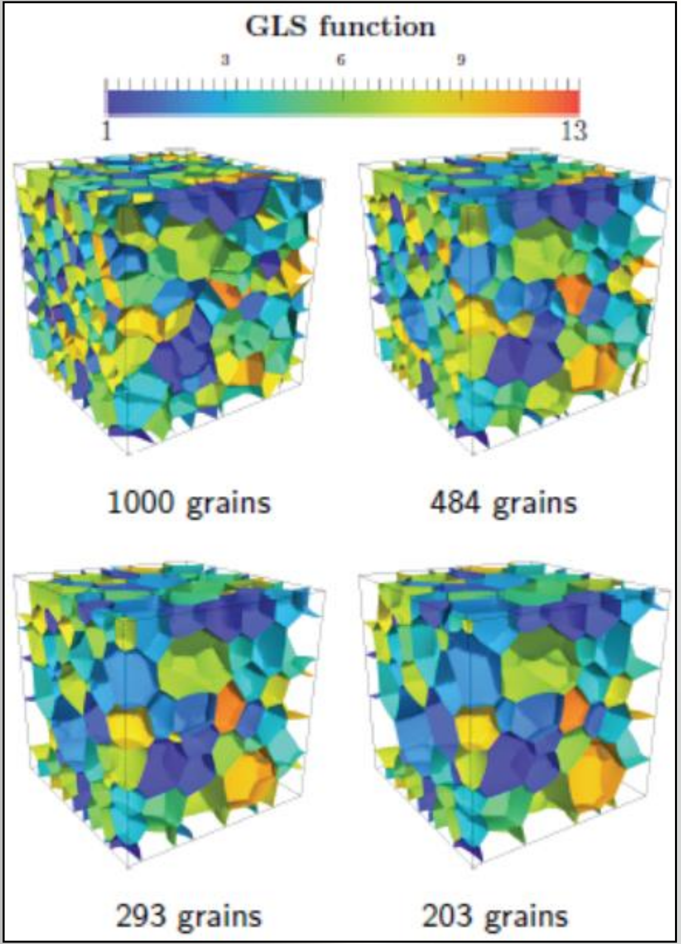
- **How to reduce computation times?**

Optimize the main steps of the computation

- Development of a new formalism for the reinitialization procedure*: the *Direct Reinitialization (DR) method*

CPU times using the initial formalism or the DR method for the reinitialization procedure





Example: 3D grain growth case (12CPUs)

- 5h of heat treatment
- Initial polycrystal composed of 1000 grains
- Material : 304L steel

[Shakoor et al., 2015]

**correction of the LS functions after an increment of computation in order to restore their metric properties*

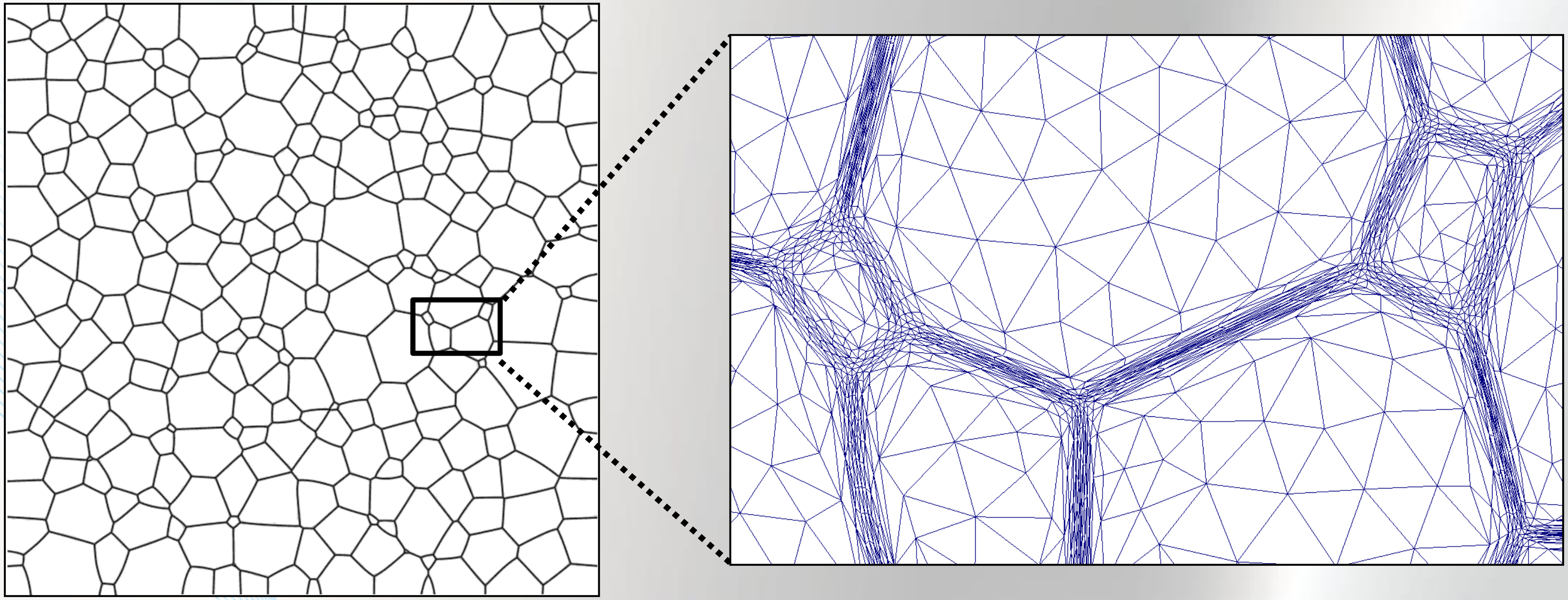
NUMERICAL IMPROVEMENTS

- **How to reduce computation times?**

Reduce the number of elements without losing precision

Realistic predictions necessitate a sharp description of the interfaces

- Use of *anisotropic mesh adaptation* (and *periodic remeshing*) around grain boundaries



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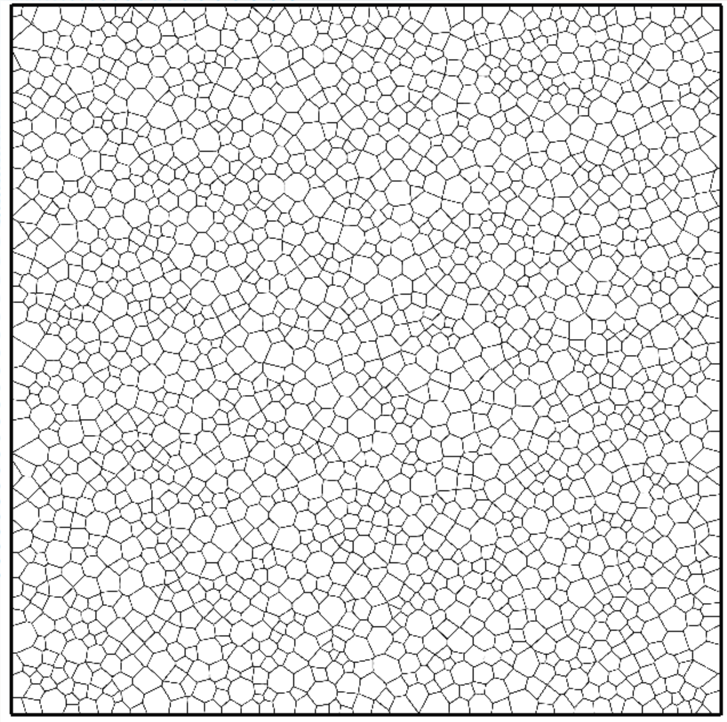
APPLICATION EXAMPLES – PURE GRAIN GROWTH

- **Solutionizing treatment in the one-phase field**



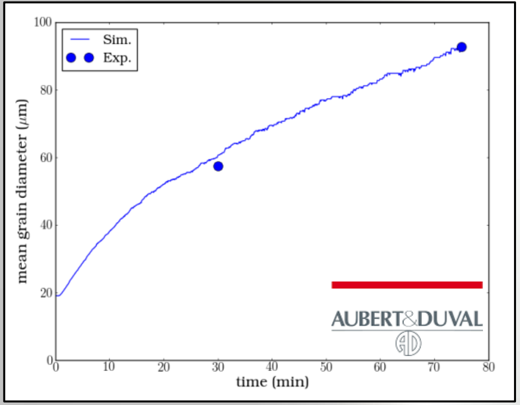
Inconel 718 heat treated 75min at 1040°C
(<d_0>=20µm, 100% γ phase)

Grain growth in monophasic structures

- ○ Microstructural evolution driven by grain boundaries (GB) curvature only (capillarity effect, no stored energy)

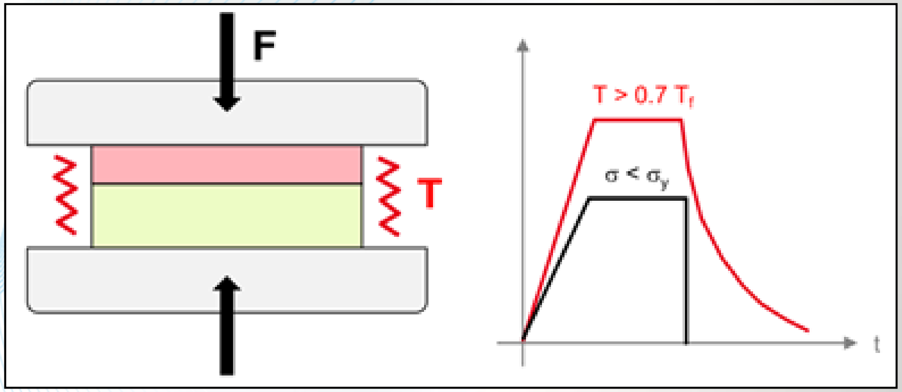
$$\begin{cases} \dfrac{\partial \psi_i(x,t)}{\partial t} - M\gamma\Delta\psi_i(x,t) + \cancel{\vec{v}_e \cdot \nabla\psi_i(x,t)} = 0, & \forall i \in \{1,\ldots,N_p\} \\ \psi_i(x,t=0) = \psi_i^0(x), \end{cases}$$

- ○ Uniform GB mobility (thermodependent)
- ○ Uniform and isotropic GB energy
- ○ Influence of initial grain size distribution

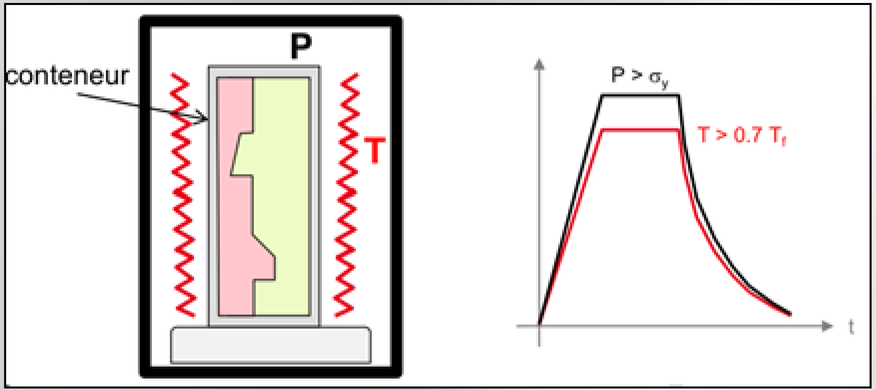


APPLICATION EXAMPLES – PURE GRAIN GROWTH

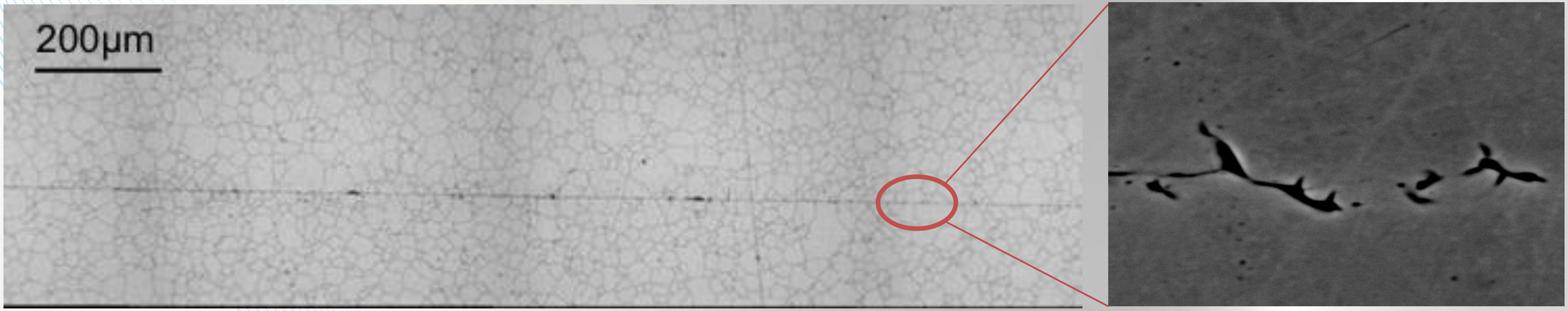
- **HIP bonding**



HIP bonding with press



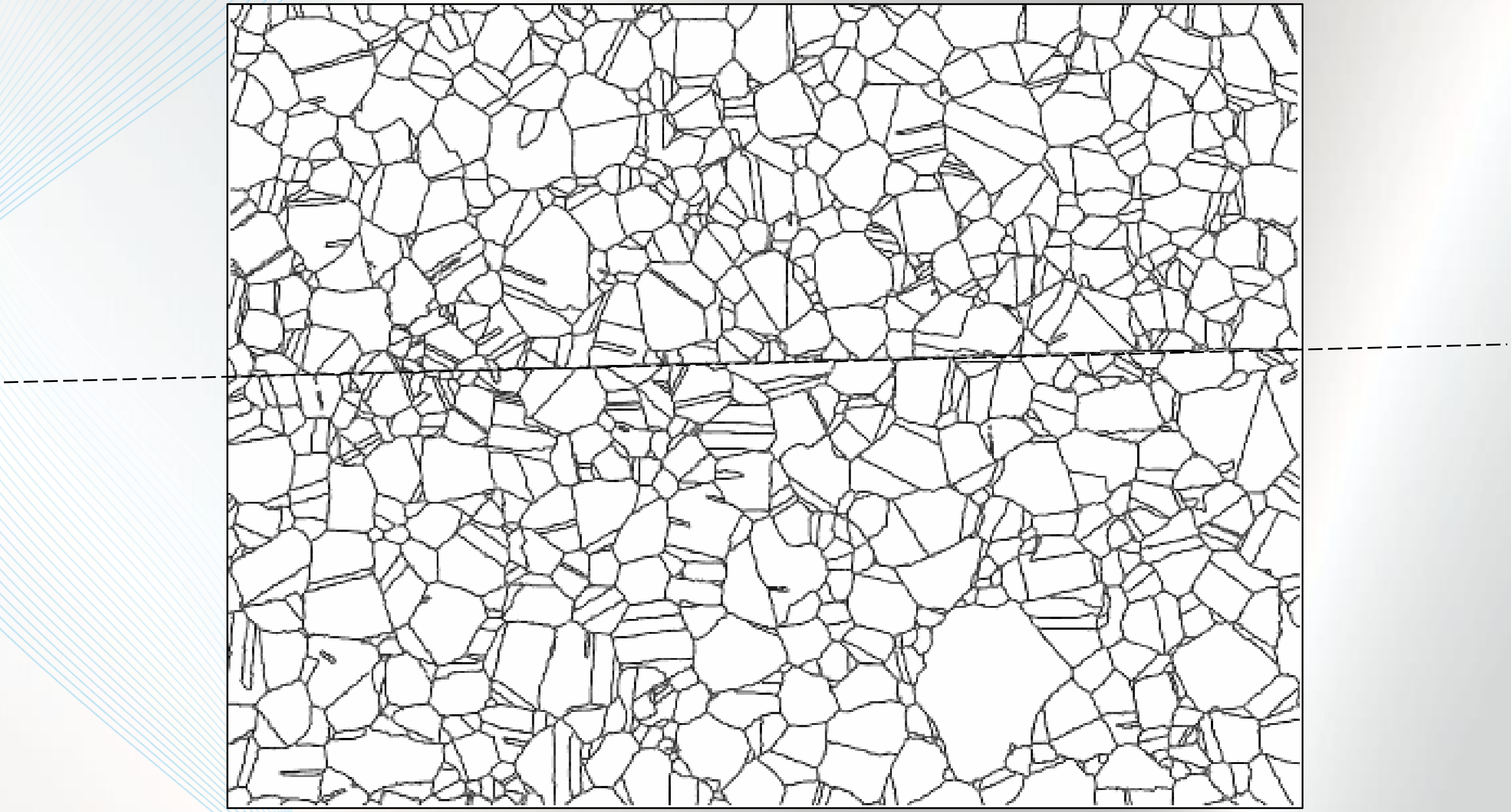
Hot Isostatic Pressing (HIP)



[E. Rigal – CEA Liten]

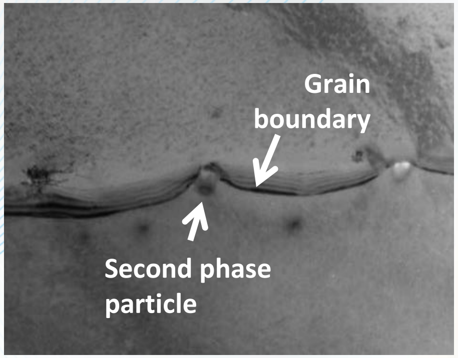
APPLICATION EXAMPLES – PURE GRAIN GROWTH

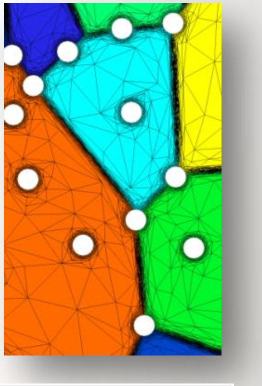
- **HIP bonding**

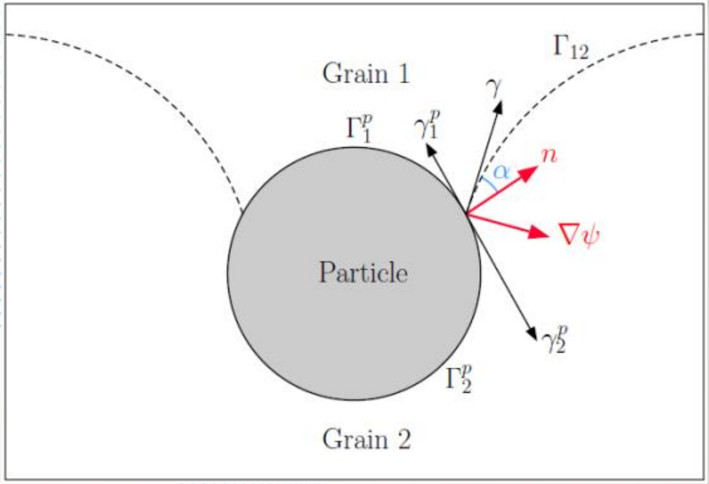


APPLICATION EXAMPLES – PRESENCE OF SPP

Smith-Zener pinning phenomenon







What is particle pinning?

- ○ Dragging force exerted by SPP on GB
  - ➔ *Slow down the GB kinetics*
  - ➔ *Enable to control the final grain size*

In LS context

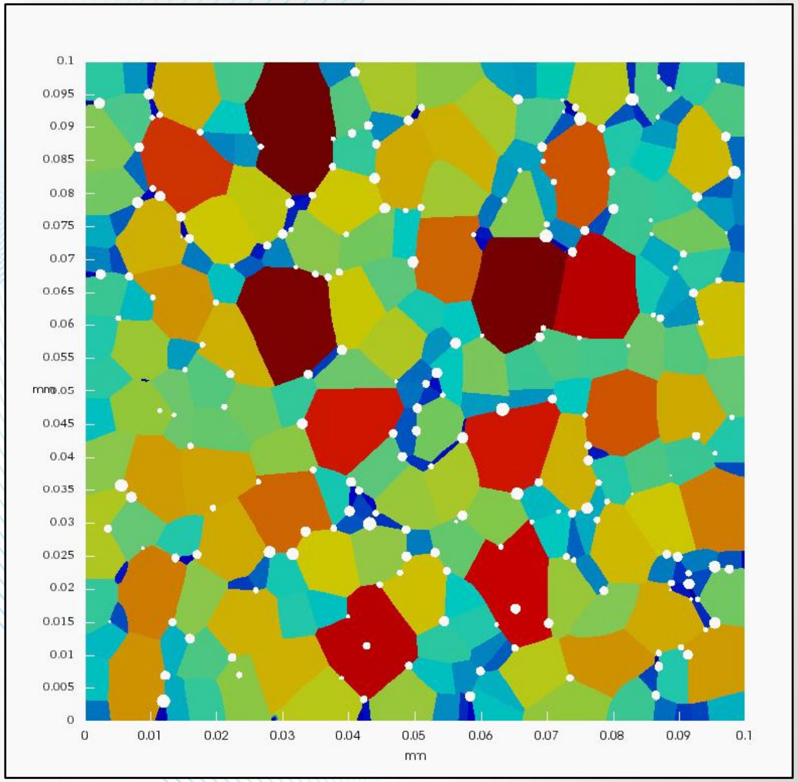
- ○ SPP explicitly represented in the FE mesh
  - ➔ *No assumptions concerning the interactions between GB and SPP*
  - ➔ *Coherent or incoherent interfaces can be considered by applying the suitable boundary conditions*

$$\boxed{\frac{\nabla\psi}{\|\nabla\psi\|}\cdot\vec{n} = \nabla\psi\cdot\vec{n} = \sin(\alpha)}$$

[Agnoli et al., 2013], [Agnoli et al., 2014], [Scholtes et al., 2015], [Scholtes et al., 2016b]

APPLICATION EXAMPLES – PRESENCE OF SPP

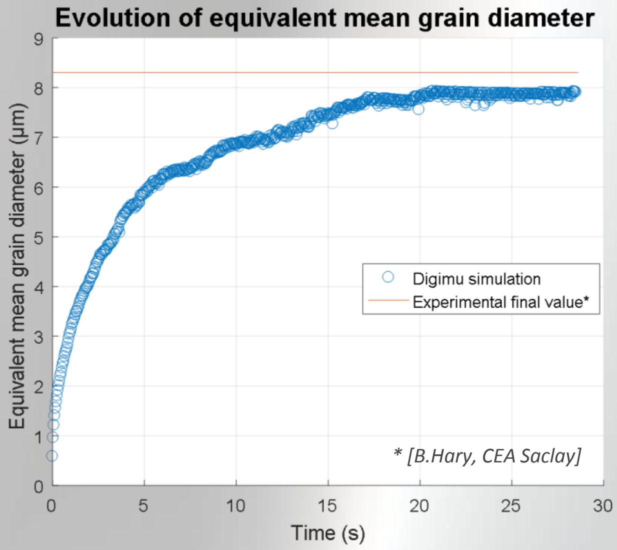
- **Control of the grain size in an ODS steel (Oxide Dispersion Strengthening)**



$\langle r_{part} \rangle$ = 600nm
f = 2,5%

[F. Villaret, B. Hary, Y. de Carlan, T. Baudin, R. Logé, M. Bernacki]

- ○ Ferritic steel + $Y_2Ti_2O_7$ nanoparticles (oxides)
- ○ Dislocations and grain boundaries pinning on the oxides

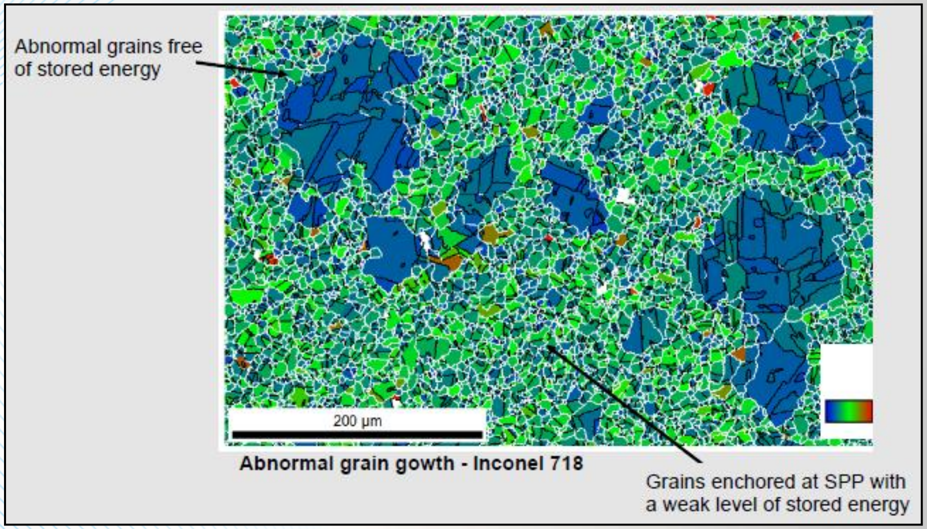


** [B.Hary, CEA Saclay]*

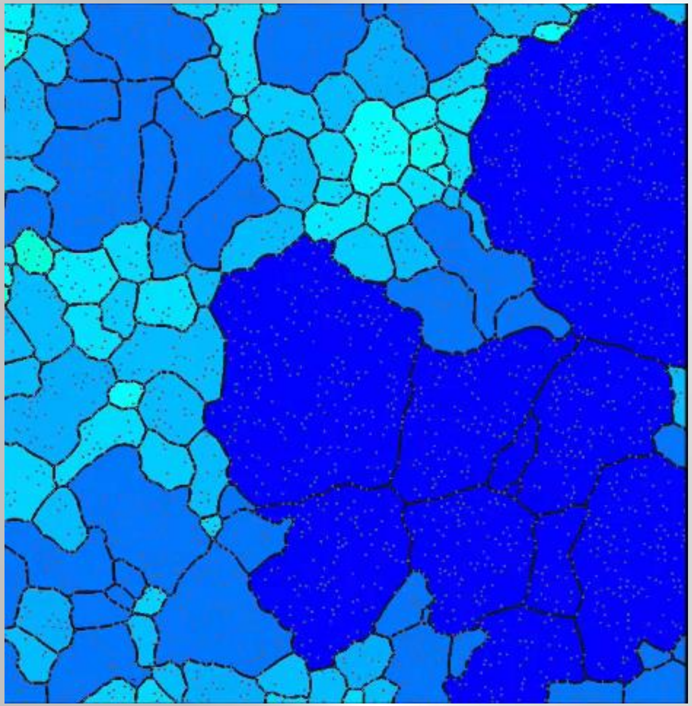
APPLICATION EXAMPLES – PRESENCE OF SPP

Understanding of the abnormal grain growth phenomenon

- Growth of a limited number of grains much faster than the rest
- Decrease of mechanical properties



Abnormal grain gowth - Inconel 718



Phenomenon controlled by the balance of: capillarity, stored-energy and pinning forces

[Agnoli et al., 2013], [Agnoli et al., 2014]

Local heterogeneity simulated implicitly

APPLICATION EXAMPLES – HOT FORMING PROCESSES

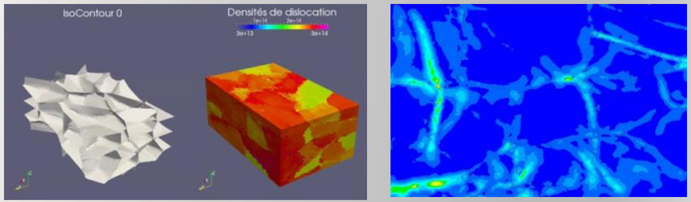
- **Modelling the different physical phenomena**

Work hardening

Recovery

Two approaches:

- Local scale with Crystal Plasticity Algorithm
  - ⚠ High computational costs for industrial applications



- Macroscopic scale with phenomenological laws

Example: Yoshie Laasraoui Jonas law $\frac{\partial \rho}{\partial \varepsilon} = K_1 - K_2\rho$ $\frac{\partial \rho}{\partial t} = -K_s\rho$

Grain boundary migration

$$\begin{cases} \frac{\partial \psi_i(x,t)}{\partial t} - M\gamma\Delta\psi_i(x,t) + \vec{v}_e \cdot \nabla\psi_i(x,t) = 0, \\ \psi_i(x,t=0) = \psi_i^0(x), \end{cases} \quad \forall i \in \{1,\dots,N_p\}$$

Nucleation of new grains

Calculation of:

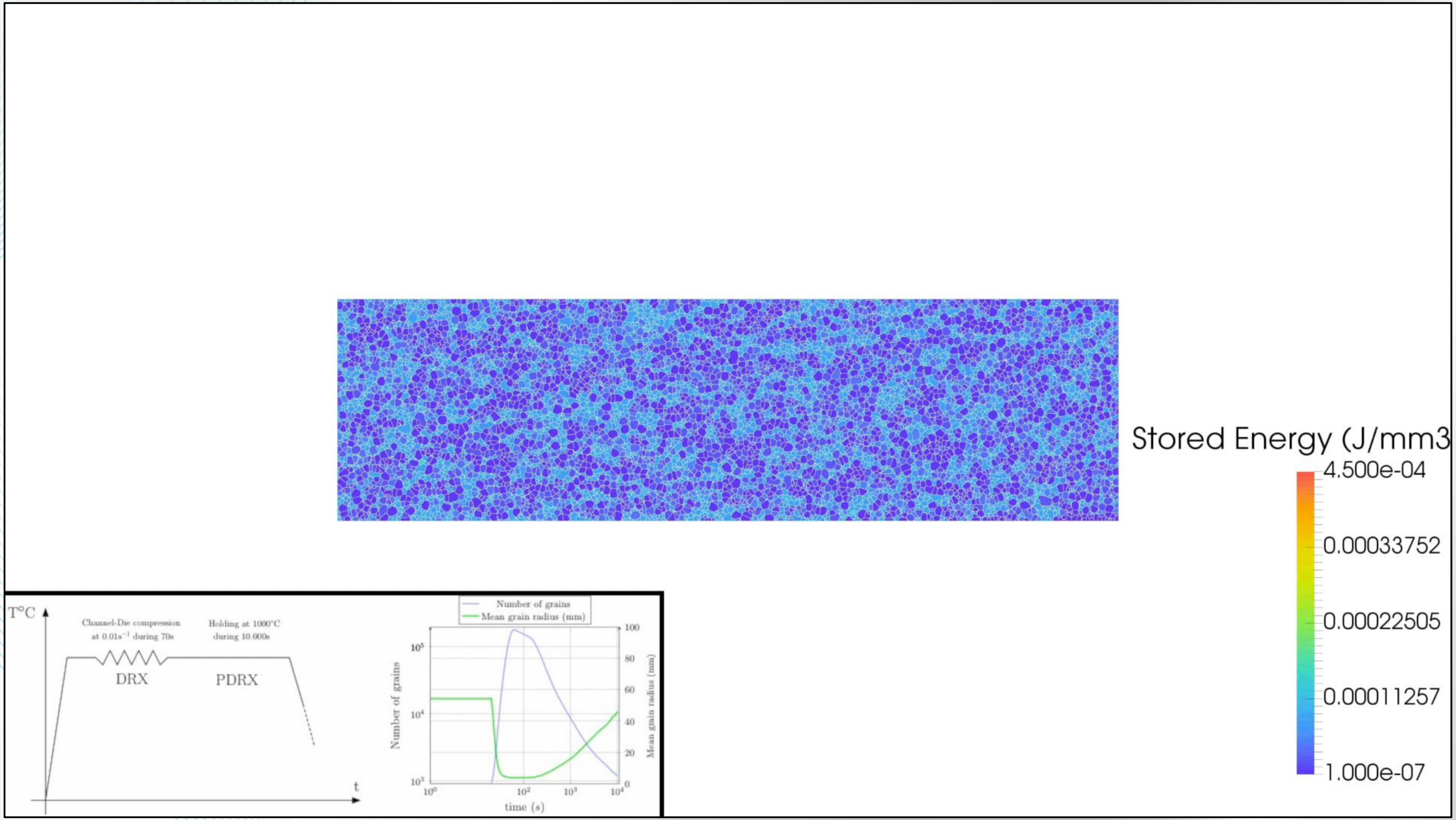
- a criterion for nucleation (ρ_{cr})
- a nucleation rate ($\dot{N}$)
- a critical nucleus size (r*)

Precipitation

[Maire et al., 2017]

APPLICATION EXAMPLES – HOT FORMING PROCESSES

- **Dynamic and Post-dynamic recrystallization**



[Maire et al., 2017]

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  - Presence of second phase particles
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CONCLUSION & PERSPECTIVES

Prediction of grain sizes evolution during thermomechanical and thermal treatments: a key for optimizing final in-use metal properties

Microstructural evolution modelling at the mesoscopic scale

- Simulate **heterogeneous** and **local** phenomena
- **Improve** mean field models for **macroscale computations**

Approach based on a Level Set description of the interfaces in a finite element framework

- Deterministic approach based on the resolution of convective-diffusive equations of the level set functions
- Grain boundary migration given by the balance of capillarity, stored-energy and pinning forces

Will to propose an industrial solution

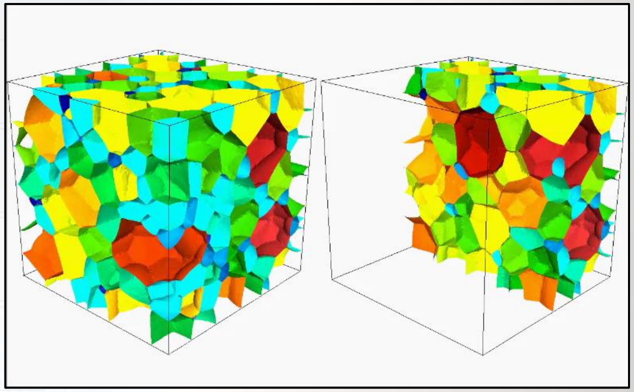
- Numerical improvements done on the method to improve computational efficiency
- Step by step introduction of the developments into the DIGIMU® software

CONCLUSION & PERSPECTIVES

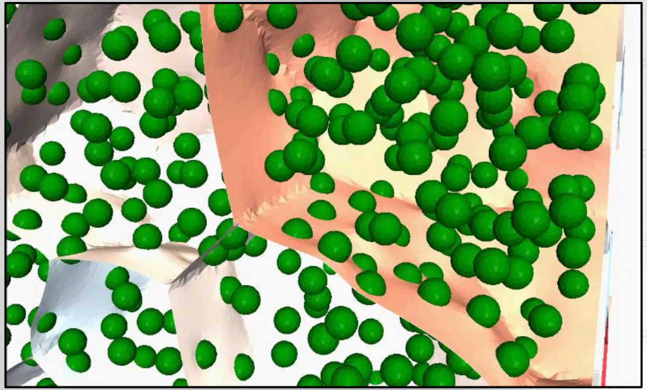
Future developments

- Continuous improvements of the physical models (anisotropy, phase transformations…)
- Towards full 3D simulations: intensive work to reduce computation times

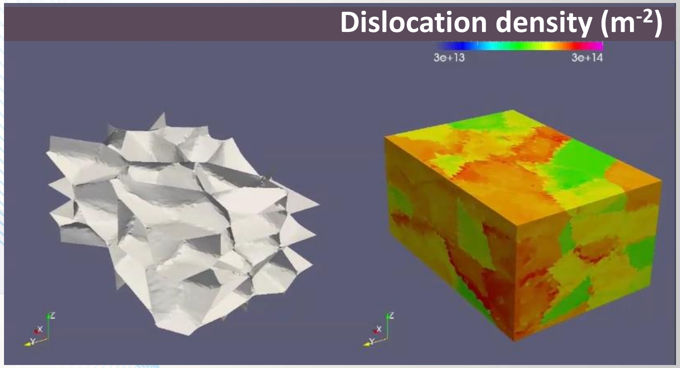
Pure grain growth[1]



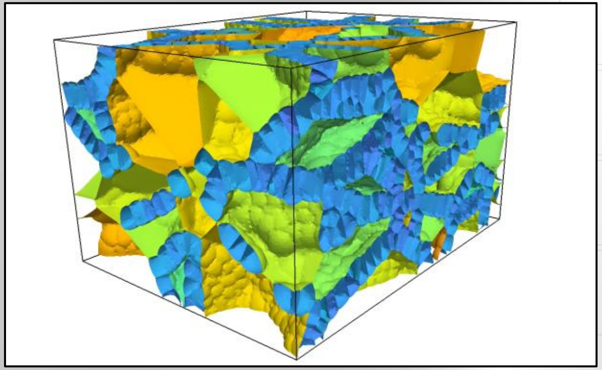
Pinning effect on second phase particles[2]



Crystal plasticity simulations (CPFEM)[3]



Dynamic and Post-dynamic recrystallization[4]



[1] [Scholtes, 2015]
[2] [Scholtes, 2016b]
[3] [Fabiano, 2014]
[4] [Scholtes, 2016a]

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