Development of an efficient level set framework for the full field modeling of recrystallization in 3D

Benjamin SCHOLTES

Supervised by: Marc BERNACKI

5 decembre 2016

Outline

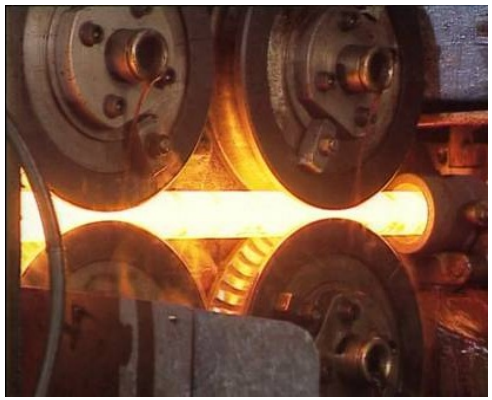
Outline

The blacksmith experience

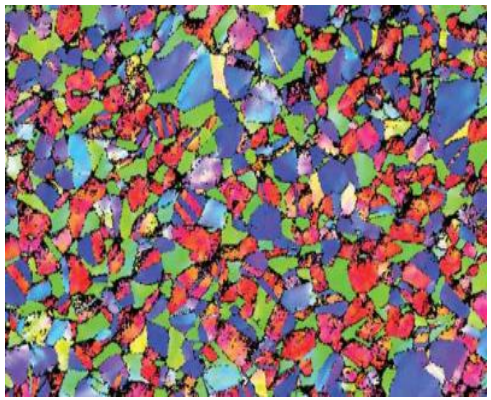
A big step forward for materials science

Introduction

Process



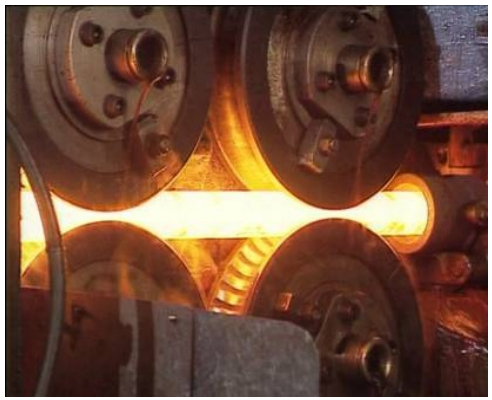
Microstructure



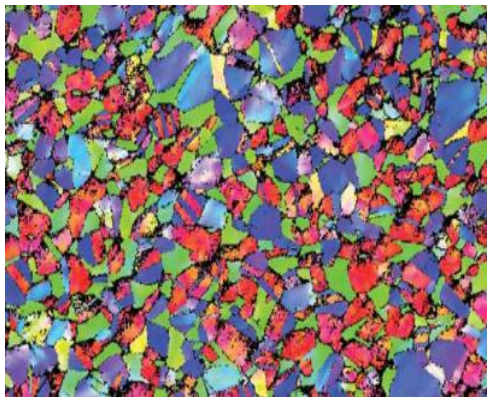
Final properties

Introduction

Process



Microstructure



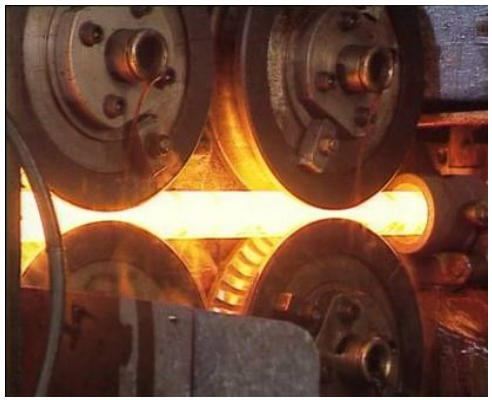
Final properties

How to predict the effects of thermo mechanical processes on microstructure?

- Experimental testing and observations
- Simulations

Introduction

Process



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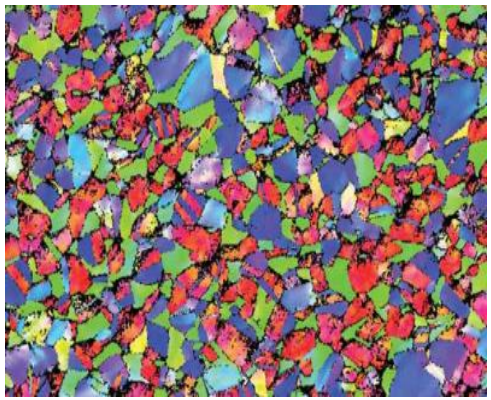
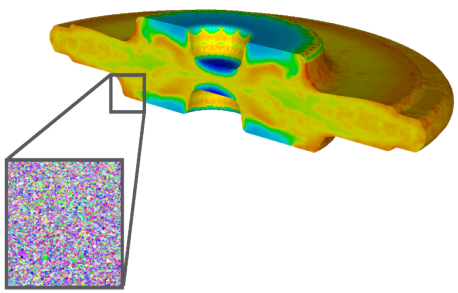


Final properties

Modeling

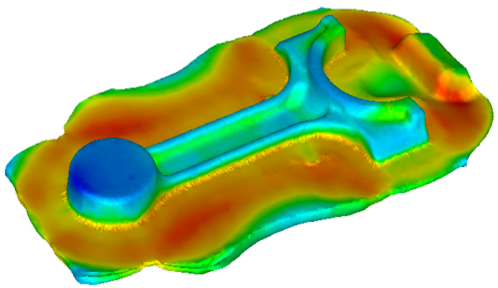


The modeling scales

Calibration ← → Prediction

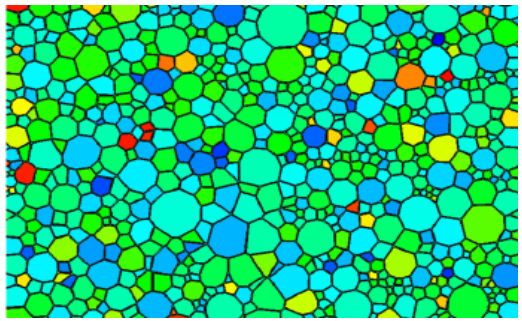
Forge® - THERMIDE — **Complex phenomena**

Macro & mean field



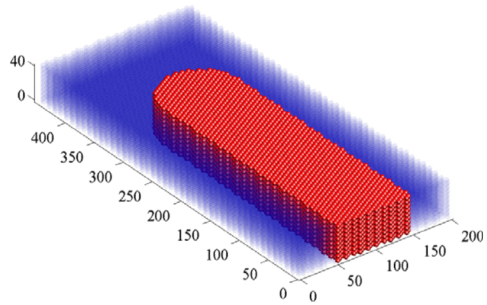
- Analytical laws (fast)
- Homogeneized quantities
- Require calibration

Meso (full field)



- Local predictions
- Versatile
- Numerical cost
- Material parameters

MD/DD models

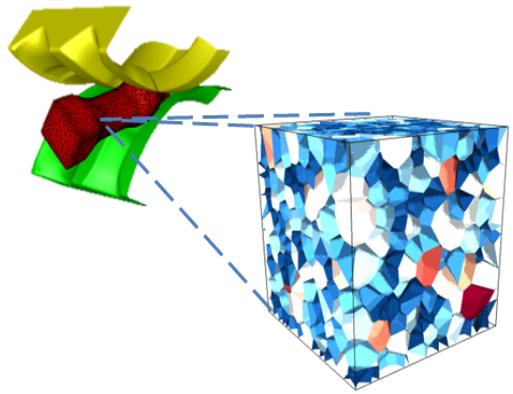


- No assumptions
- Prohibitive costs
- Parameters

Boundary conditions ↑ Material parameters

Development of multiscale strategies

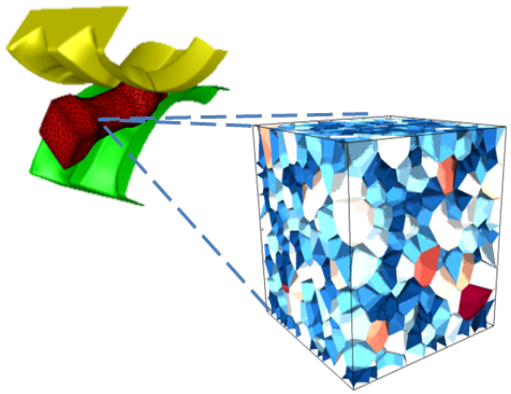
Macro $\rightarrow$ Mean field $\rightarrow$ Micro



- Coupling with macroscopic codes

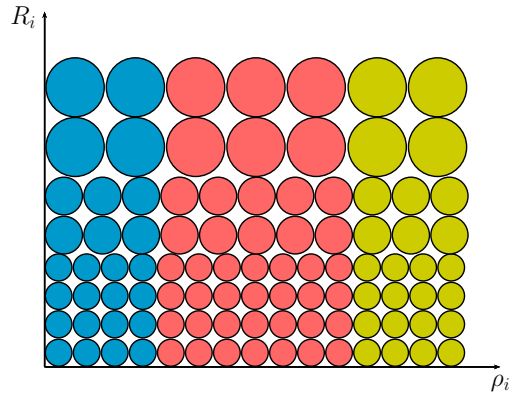
Development of multiscale strategies

Macro → Mean field → Micro



- Coupling with macroscopic codes

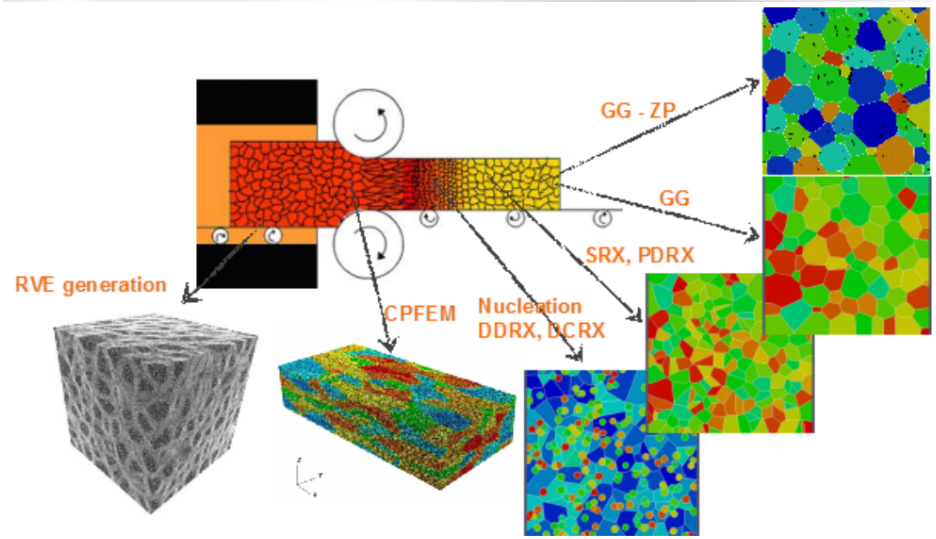
Micro → Mean field → Macro



- Toolbox for upper-scale models

Development of a commercial solution: DIGIMU software

DIGIMU® 1.0 by Transvalor



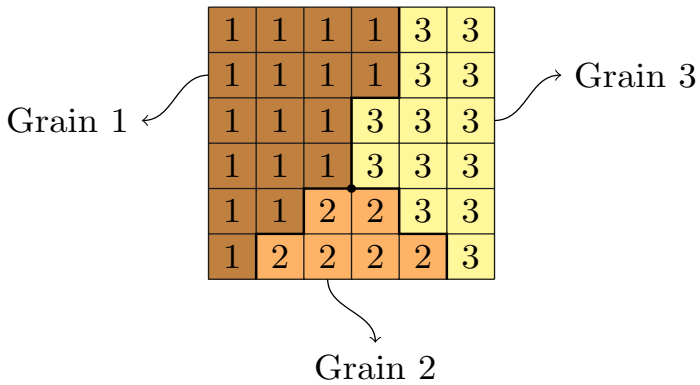
To attract industrials, DIGIMU must be:

- **Versatile**
- **Numerically efficient** and **robust**

MINES ParisTech · Cemef · AUBERT&DUVAL · cea · AREVA · ArcelorMittal · ASCOMETAL · SAFRAN AEROSPACE · DEFENCE · SECURITY · TIMET TIMET Savoie S.A. · TRANSVALOR

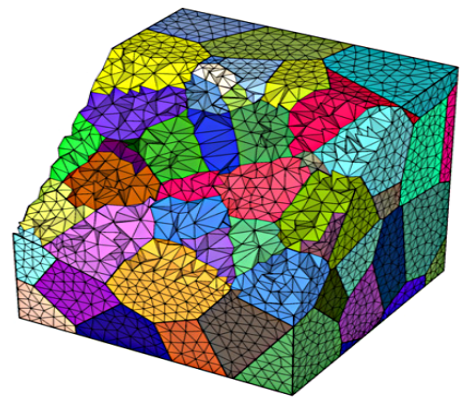
Full field approaches for the modeling of ReX and GG

Stochastic approaches (MC, CA)



- Fast and well-suited with parallelization
- Easy implementation
- Coupling with other methods to handle large polycrystal deformations (industrial applications)

Deterministic approaches (Vertex, PF, LS)



- Deterministic evolution laws
- Allow finite element formulations
- Numerical cost

Full field approaches for the modeling of ReX and GG

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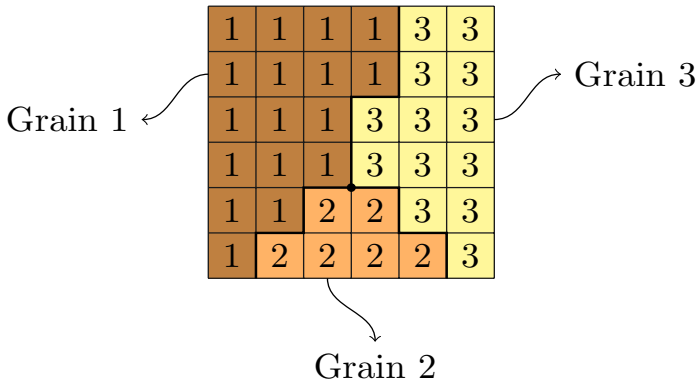

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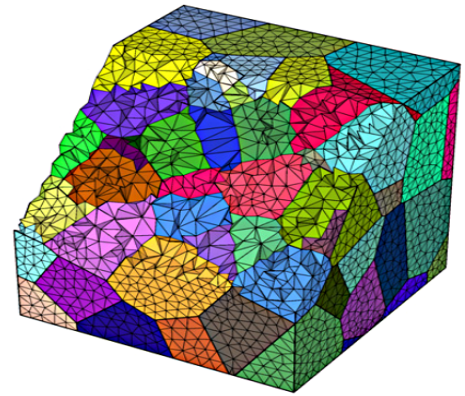

Our choice? Using a level set (LS) approach within a finite element (FE) framework

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Steinbach et al. "A generalized field method for multiphase transformations using interface fields" *Physica D* (1999)

Rollett et al. "A hybrid model for mesoscopic simulation of recrystallization" *Comp. Mat. Sci.* (2001)

Logé et al. "Linking plastic deformation to recrystallization in metals using digital microstructures" *Phil. Mag.* (2008)

Hallberg et al. "Simulation of discontinuous dynamic recrystallization in pure Cu using a probabilistic cellular automaton" *Comp. Mat. Sci.* (2010)

Bernacki et al. "Level set framework for the finite-element modelling of recrystallization and grain growth in polycrystalline materials" *Scripta Mat.* (2011)

Madej et al. "Multi scale cellular automata and finite element based model for cold deformation and annealing of a ferritic-pearlitic microstructure" *CMS* (2013)

Mellbin et al. "A combined crystal plasticity and graph-based vertex model of dynamic recrystallization at large deformations" *MSMSE* (2015)

The LS/FE approach, but why?

Allows to model most metallurgical phenomena (polycrystal deformation, twin boundaries, CPFEM, dislocation dynamics,...) in **a unified and consistent numerical framework** $\rightarrow$ versatility

The needed simulation parameters are measurable quantities that have a direct physical interpretation

CEMEF has an extensive experience in FE formulation and many numerical tools already available (stabilized FE solvers, anisotropic remeshing algorithms,...)

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Require important efforts for the implementation

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High computational cost

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Require important efforts for the implementation

High computational cost $\rightarrow$ main objective of this thesis work

Improvement of numerical efficiency: which strategy?

Size of the polycrystals

- Use of periodic boundary conditions

No size effects

Small number of grains

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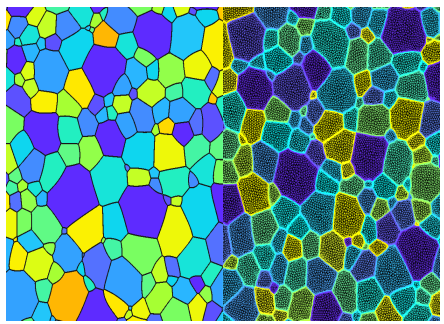
Remeshing and HO methods



- Improvement of the remeshing techniques


Less DOFs, better simulations times


Precision

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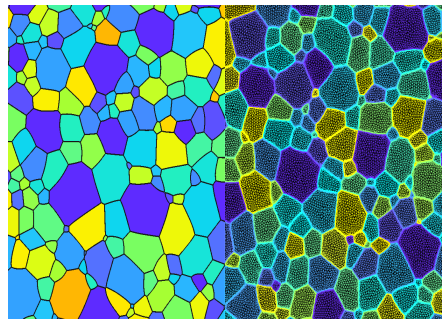

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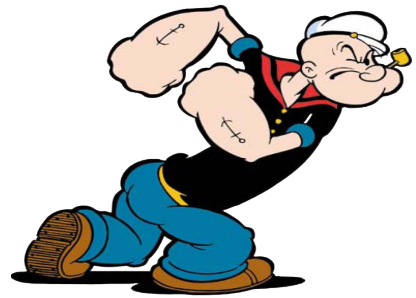
"Brutal" approach



- Optimization of the full field formalism


Developments are generic (don't be selfish!)


Better robustness and flexibility

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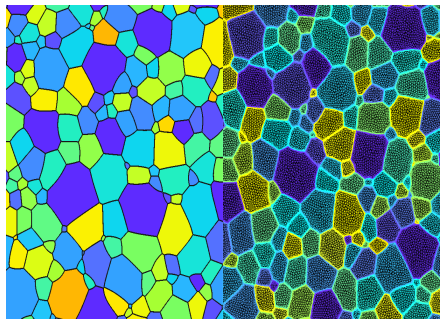
Remeshing and HO methods



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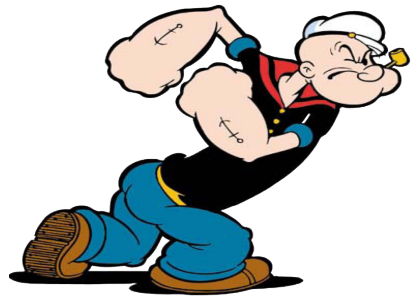

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Outline

The level set (LS) method

LS function

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

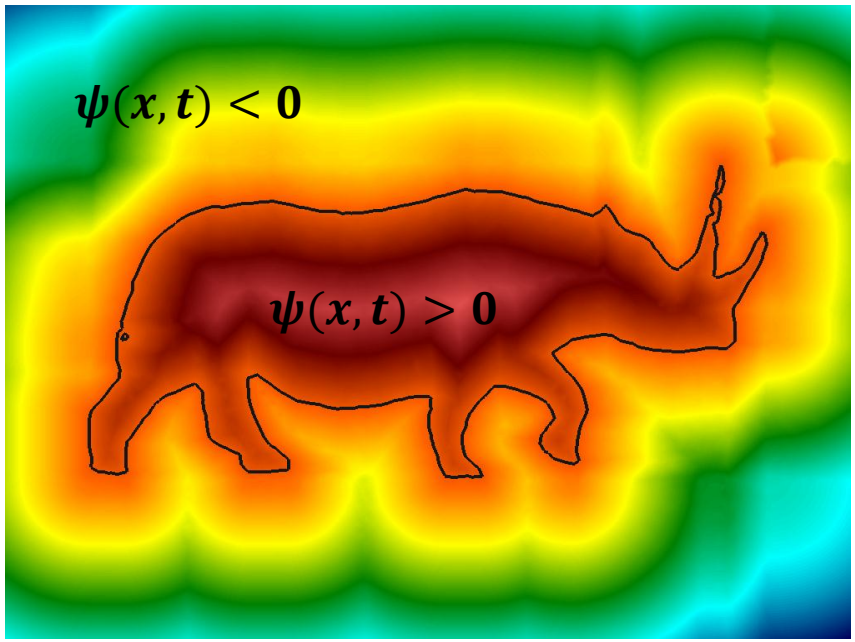
Displacement of the GLS interfaces

$$\begin{cases} \dfrac{\partial \psi}{\partial t} - M\gamma\Delta\psi + \vec{v}^e \nabla\psi = 0 \\ \psi(x, t=0) = \psi^0(x) \end{cases}$$

Reinitialization of the distance function

- How to restore the metric property?

$$\|\nabla\psi\| = 1$$



Distance function of a rhino

Osher & Sethian "Fronts propagating with curvature-dependent speed : Algorithms based on Hamilton-Jacobi formulations" *Journal of Comp. Phys.* (1988)

Bernacki et al. "Level set framework for the numerical modelling of primary recrystallization in polycrystalline materials" *Scripta Mat.* (2008)

Bernacki et al. "Level set framework for the finite-element modelling of recrystallization and grain growth in polycrystalline materials" *Scripta Mat.* (2011)

To a massively multi-domain context

REV generation

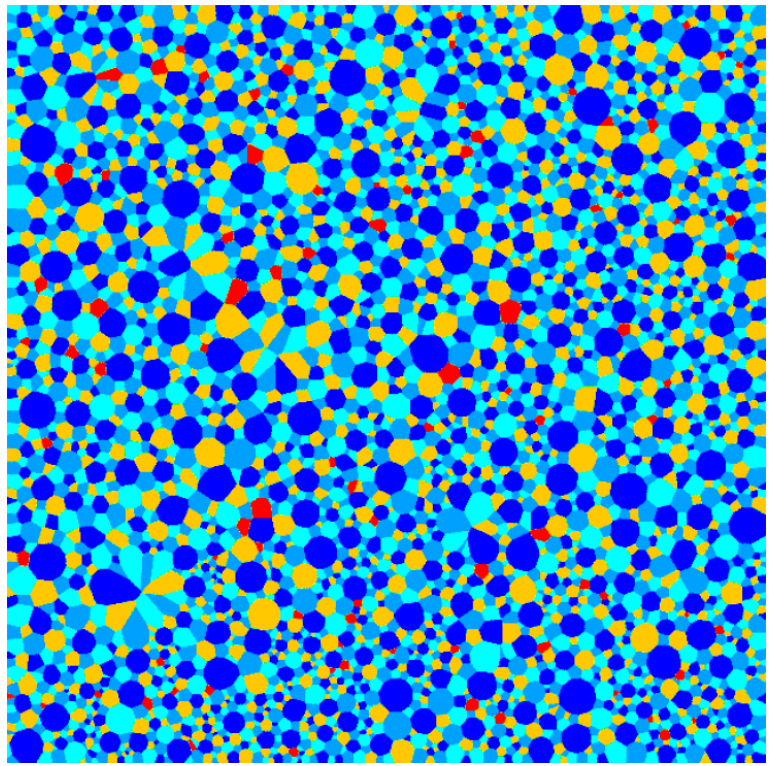
- Methods of Voronoi, Laguerre-Voronoi or immersion of an experimental image
- Respect a prescribed equiaxial grain size distribution

Complexity of representing large polycrystals

- All numerical costs of the simulations (except remeshing) depend strongly on the number of LS functions

Grain coloring

- A set of initially distinct grains can be packed in a single LS function $\rightarrow$ Global level set (GLS functions)



Microstructure composed of 3680 grains respecting a prescribed GS distribution and represented by 5 GLS functions

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Telley et al. "The Laguerre model of grain growth in two dimensions I. Cellular structures viewed as dynamical Laguerre tessellations" *Phil. Mag.* (1996)

Wu et al. "Analysis of a sector crack in a three-dimensional Voronoi polycrystal with microstructural stresses" *Journal of App. Mech.* (2000)

Hitti et al. "Precise generation of complex statistical Representative Volume Elements (RVEs) in a finite element context" *Comput. Mater. Sci.* (2012)

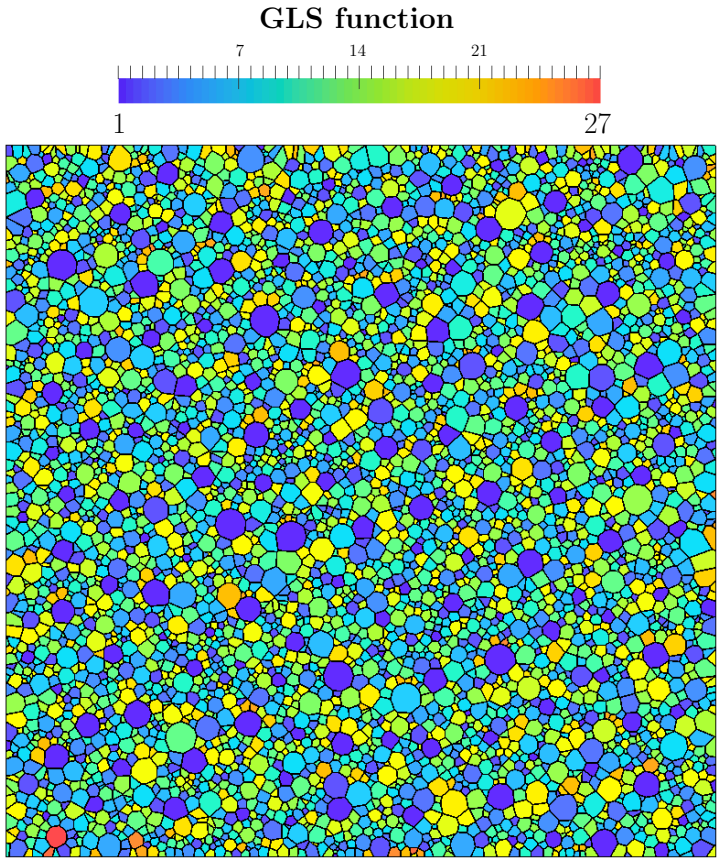
Main limitations (1): numerical cost

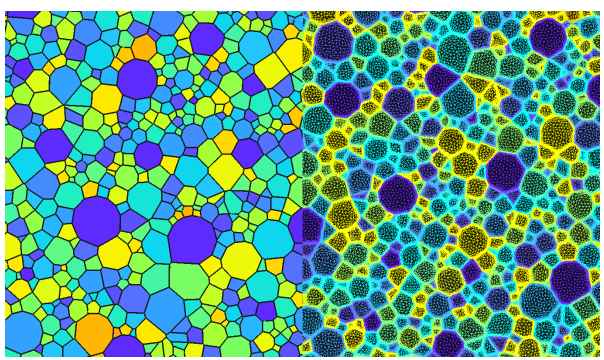
A simple grain growth case

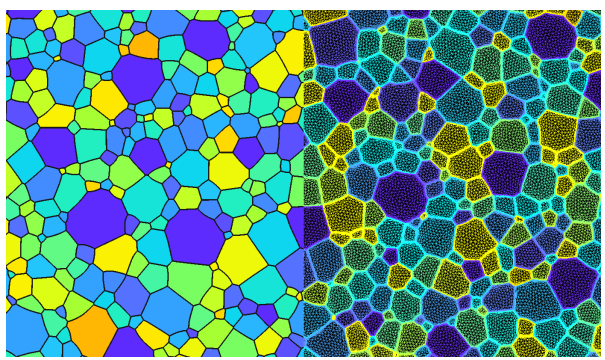
- 5h of heat treatment at 1050°C
- Initial polycrystal composed of 5000 grains
- Material : 304L austenitic steel

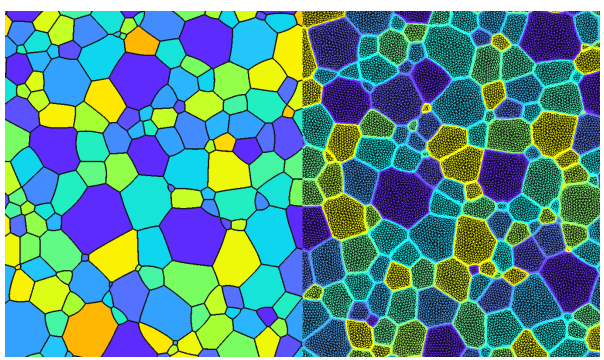
Time distribution

- 66h of computations on 6 Xeon CPUs distributed as followed:
  - 6.4% for the resolution of PDEs
  - 89.8% for reinitialization
  - 3.1% for remeshing
  - 0.7% for post-treatment operations

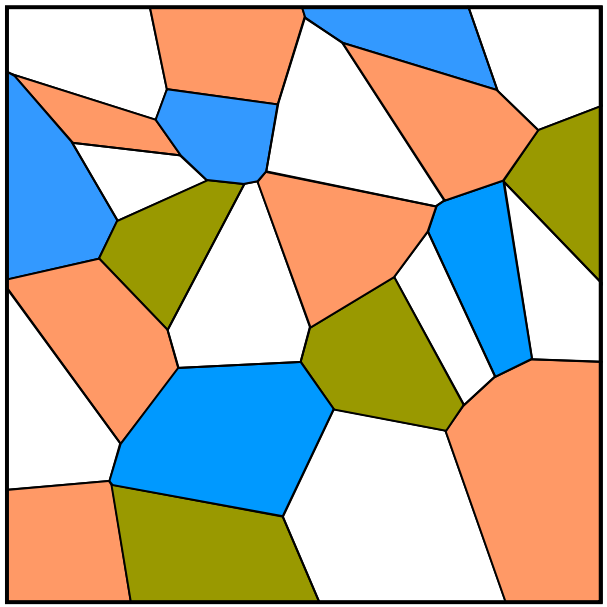




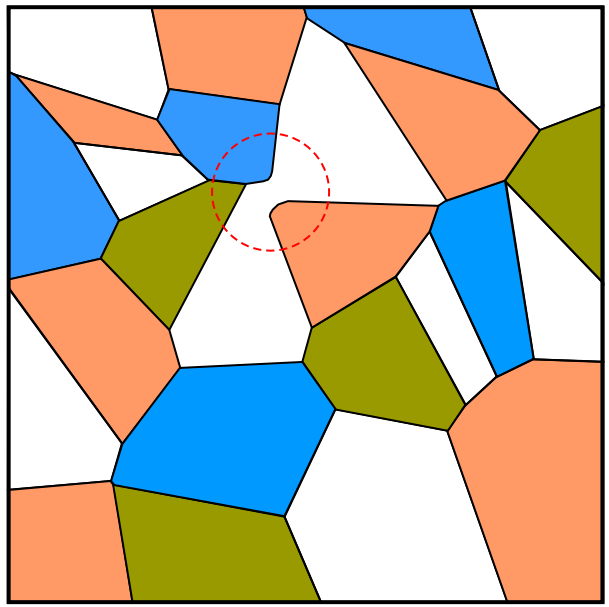




Main limitations (2): possibility of coalescence



25 grains represented by 4 colors



Coalescence

Problem statement

How to avoid coalescence by keeping an almost minimal number of GLS functions?

New developments and improvements

- A new efficient and parallel reinitialization method
- Implementation of an algorithm enabling to recolor dynamically the grains during the coalescence to avoid coalescence events and to keep a low number of GLS functions in the same time
- Development of a new formalism for ReX simulation taking advantage of the previous developments
- Improvement of the numerical approach for the modeling of microstructural evolution with inert second phase particles

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M. Shakoor, B. Scholtes, P.-O. Bouchard, M. Bernacki "An efficient and parallel level set reinitialization method - Application to micromechanics and microstructural evolutions, *Applied Mathematical Modelling* (2015)

B. Scholtes, M. Shakoor, A. Settefrati, P.-O. Bouchard, N. Bozzolo, M. Bernacki "New finite element developments for the full field modeling of microstructural evolutions using the level set method", *Computational Materials Science* (2015)

B. Scholtes, R. Boulais-Sinou, A. Settefrati, D. Pino Munoz, I. Poitrault, A. Montouchet, N. Bozzolo, M. Bernacki "3D level set modeling of static recrystallization considering stored energy fields", *Computational Material Science (2016)*

B. Scholtes, D. Ilin, A. Settefrati, N. Bozzolo, A. Agnoli, M. Bernacki "Full field modeling of the Zener pinning phenomenon in a level set framework - discussion of classical limiting mean grain size equation", *Proceedings of Superalloys 2016 : The 13th international symposium on superalloys (2016)*

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Old approach for GLS function reinitialization

Hamilton-Jacobi (HJ) method

$$\begin{cases} \dfrac{\partial \psi^*}{\partial \tau} = sgn(\|\nabla \psi^*\| - 1) \\ \psi^*(x, \tau = 0) = \psi(x, t) \end{cases}$$

- Quite versatile
- Iterative (long...) but enables a full reinitialization
- Numerical time step (calibration) and stabilization parameters

---

Sussman et al. "A level set approach for computing solutions to incompressible two-phase flow" *Journal of Computational Physics* (1994)

Coupez "Convection of local level set function for moving surfaces and interfaces in forming flow" *AIP Conference Proceedings* (2007)

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Conclusions about the HJ method

This reinitialization approach has been proven very ineffective for our applications, because:

- One works with an elevated number of GLS functions (even with coloring)
- The initial GLS functions are extremely irregular due to the treatment performed after transport, making them hard to reinitialize by a non-direct approach

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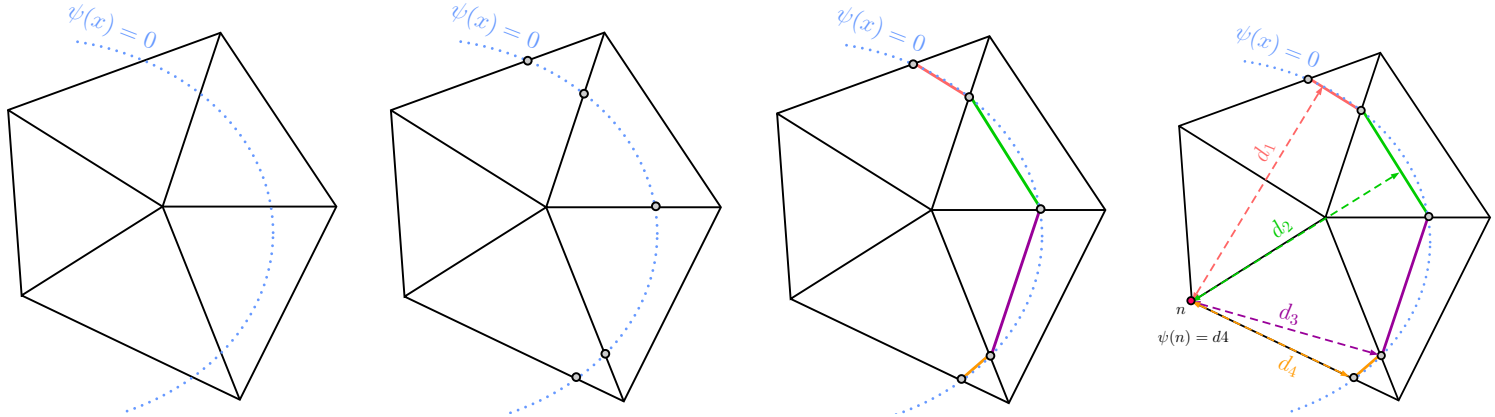
Coupez "Convection of local level set function for moving surfaces and interfaces in forming flow" *AIP Conference Proceedings* (2007)

Direct reinitialization (DR) method



Basic concept

- Find intersection between the contour and the edge through interpolations
- Construct a local discretized contour **and broadcast to other processors**
- Update the value of the LS function by computing the distance **to each of** the elements of the discretized contour and taking the shortest

M. Shakoor, B. Scholtes, P.-O. Bouchard, M. Bernacki "An efficient and parallel level set reinitialization method - Application to micromechanics and microstructural evolutions", *Applied Mathematical Modelling* (2015)

The DR approach: advantage and limitations

- Analytical reconstruction (exact)
- No numerical parameter
- Conservative
- Robust
- Gain of one derivation order (exact P1 gradient)
- High computational cost $\rightarrow \mathcal{O}(c)$, where c is the number of facets in the piecewise linear contour

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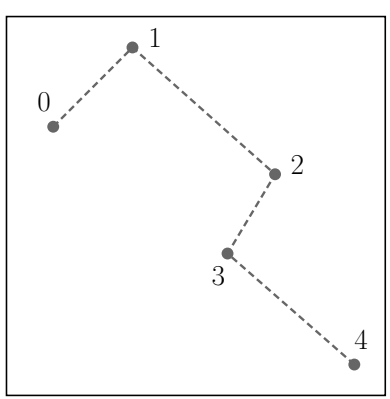
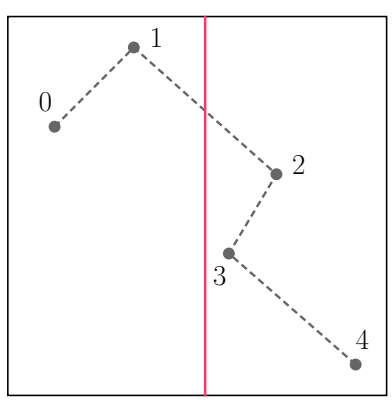
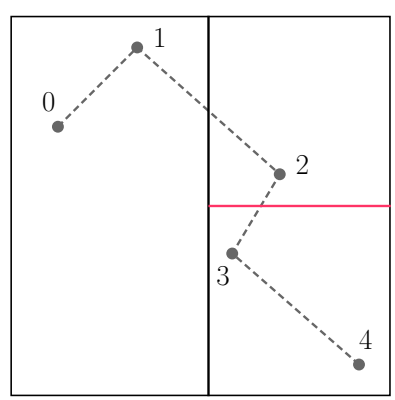
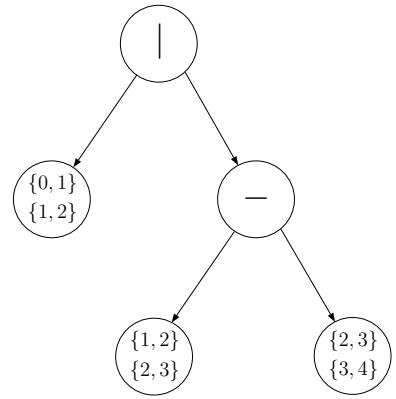
Interesting but not sufficient: we want to have your cake (inherent advantages of the DR method) and eat it (low simulation times)!
$\rightarrow$ Developement of the DR with Trees (DRT) method

The DRT method







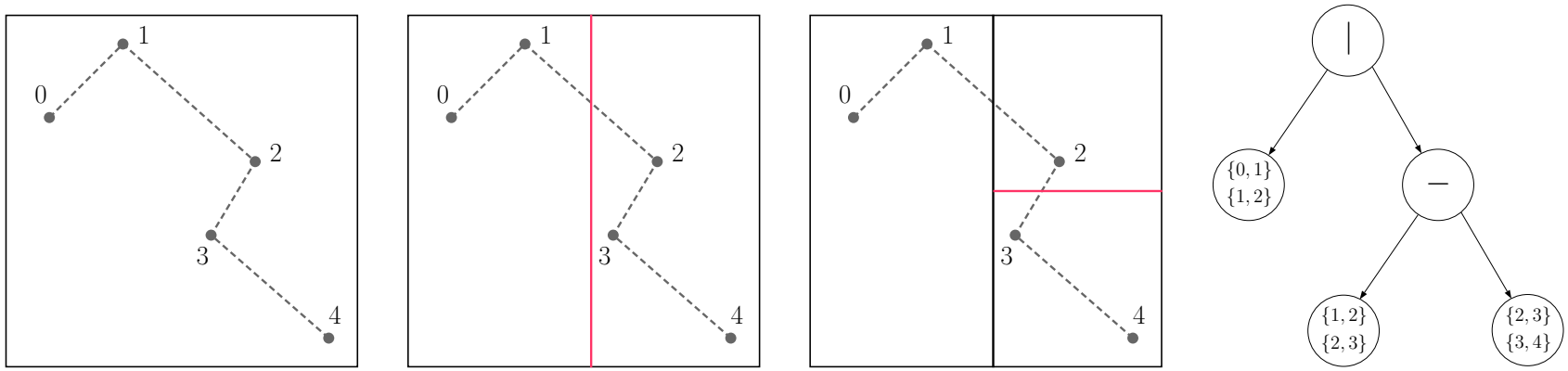


Basic concept

- A k-d tree is a space-partioning data structure for organizing points in a k-dimensional space
- On average, the complexity of a search in a k-d tree is $\mathcal{O}(\log c) << \mathcal{O}(c)$ and equal to $\mathcal{O}(c)$ in the worst case (extremely rare)

M. Shakoor, B. Scholtes, P.-O. Bouchard, M. Bernacki "An efficient and parallel level set reinitialization method - Application to micromechanics and microstructural evolutions" *Appl. Math. Model.* (2015)

The DRT method



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In parallel $\rightarrow$ recovery of the maximal efficiency

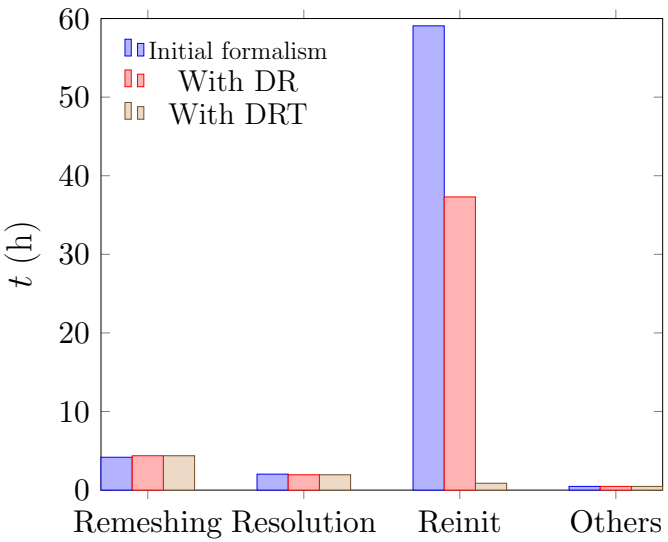
- A k-d tree and its respective bounding box are constructed independently on each process
- Other processes are interrogated **only if** they can improve the solution found at the local level (on the current partition)

M. Shakoor, B. Scholtes, P.-O. Bouchard, M. Bernacki "An efficient and parallel level set reinitialization method - Application to micromechanics and microstructural evolutions" *Appl. Math. Model.* (2015)

Improvement of simulation time for 2D simulation

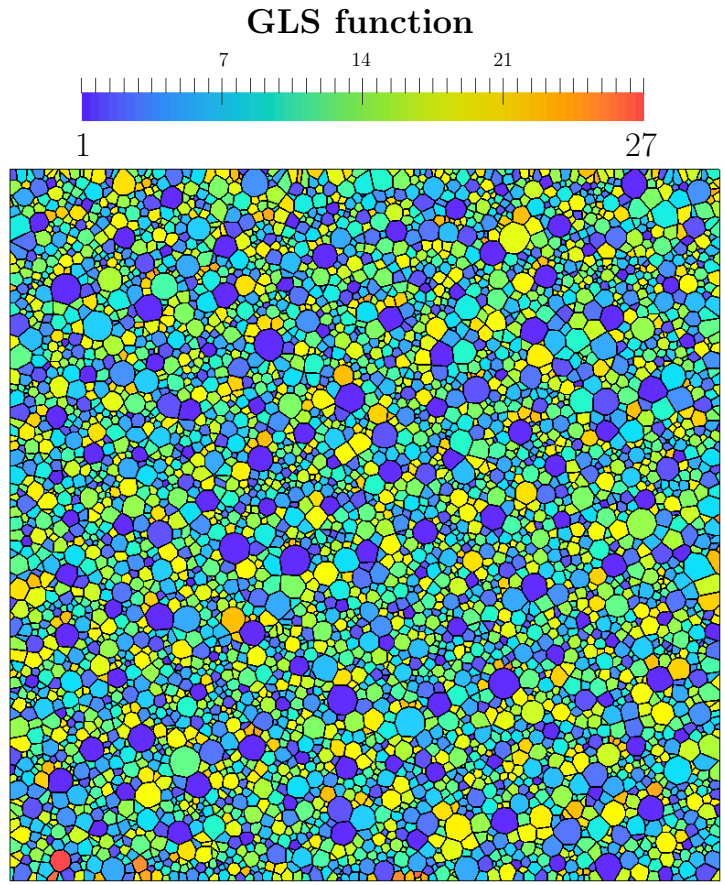
A simple 2D grain growth case (6 CPUs)

- 5h of heat treatment at 1050°C
- Initial polycrystal composed of 5000 grains
- Material : 304L austenitic steel



With DR: acceleration factor → 1.5

With DRT: acceleration factor → 9



Initial 2D polycrystal (5000 grains)

First 3D simulation

A simple 3D grain growth case (12 CPUs)

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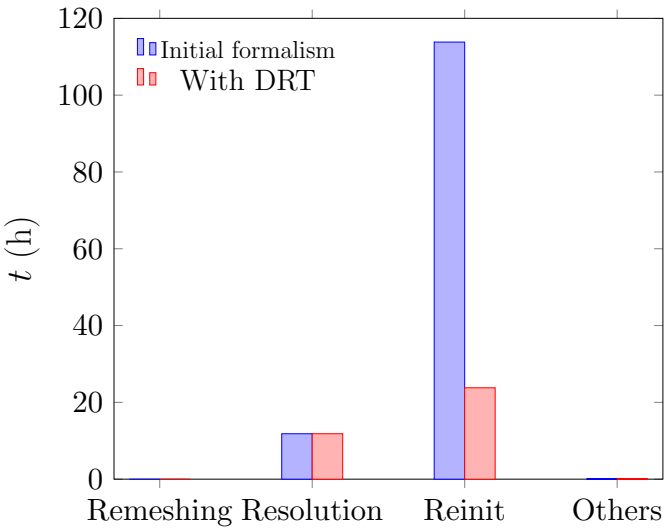
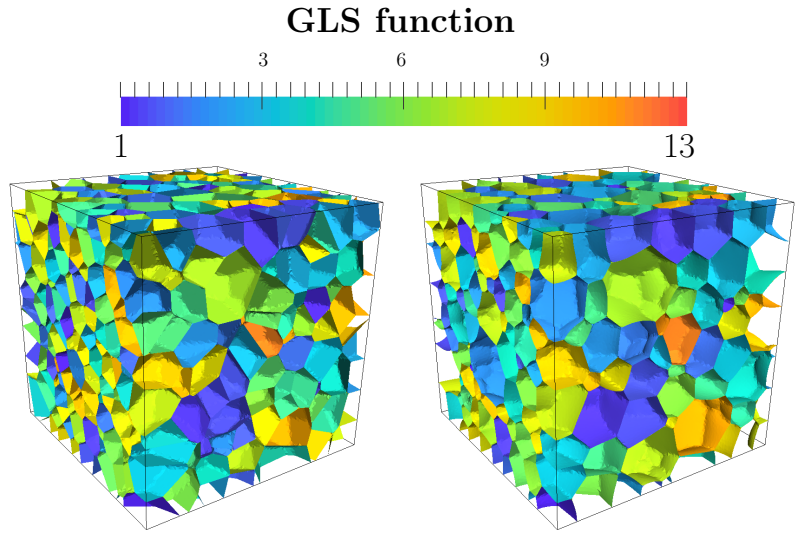
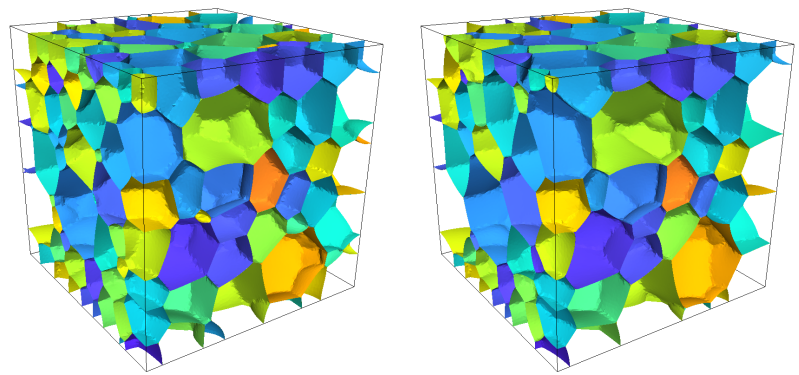


With DRT: acceleration factor → 3.5



1000 grains

484 grains

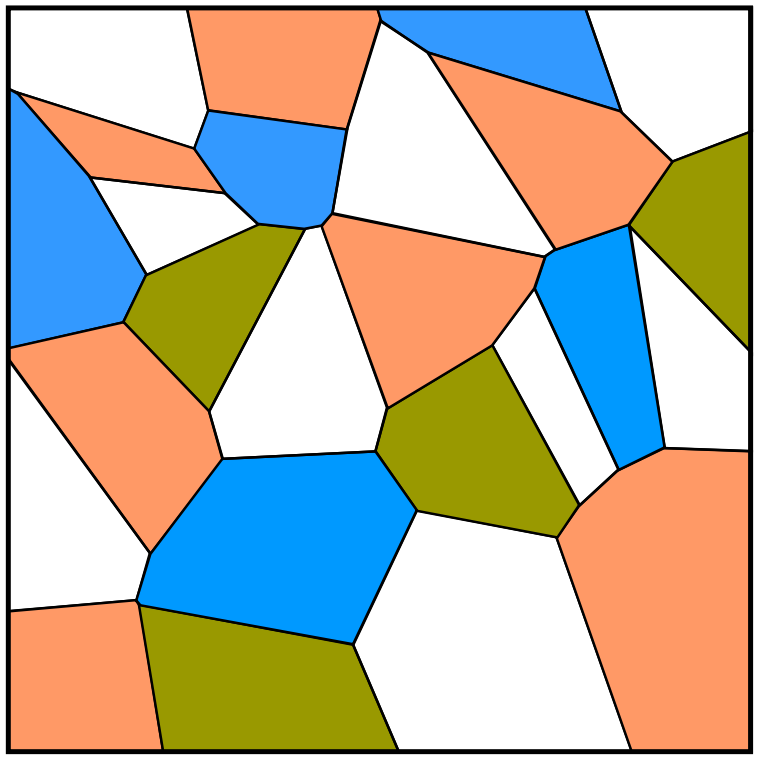


293 grains

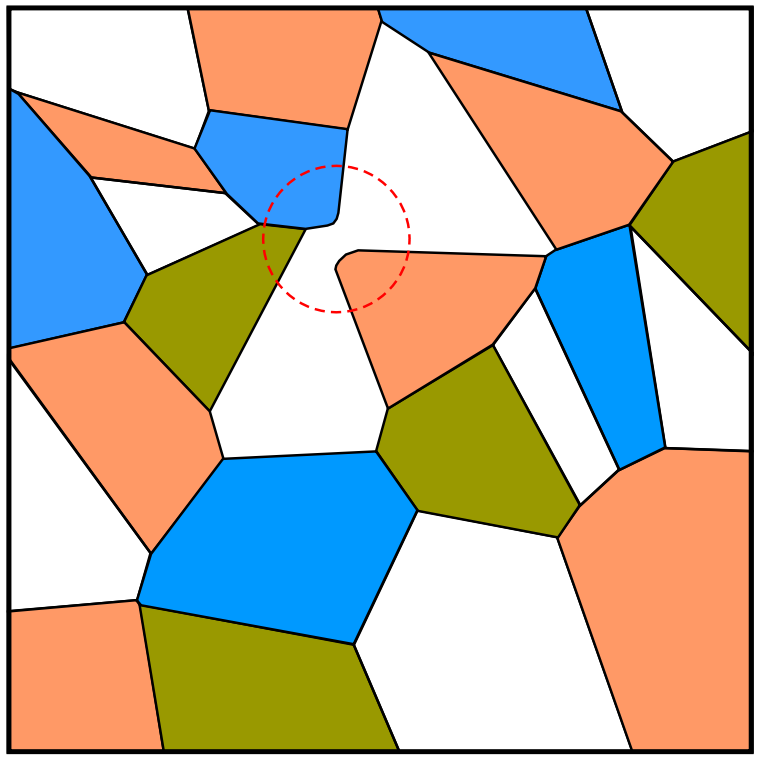
203 grains

Outline

Coalescence



25 grains represented by 4 colors



Coalescence

Problem statement

How to avoid coalescence by keeping an almost minimal number of GLS functions?

Objectives

What are we looking for?

- Prevent coalescence
- Limit the number of GLS functions to a minimum (reduction of the numerical cost)
- Propose a turnkey solution for the user without parameter or calibration

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- Systematic
- Fast
- Smart handling of the colors

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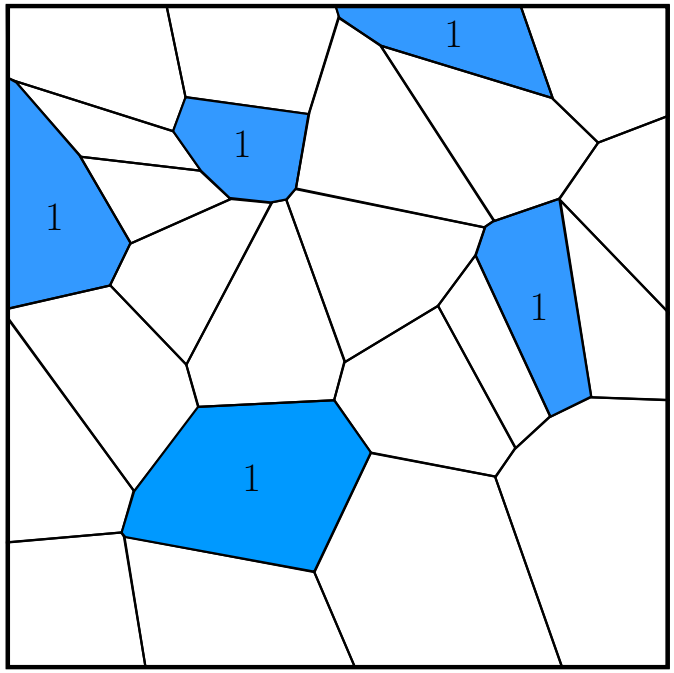
The steps of the algorithm

- Separation of the connected components
- Detection and treatment of the coalescence risks

Separation of the connected components (SCC)



Characteristic field of a GLS function containing 5 grains

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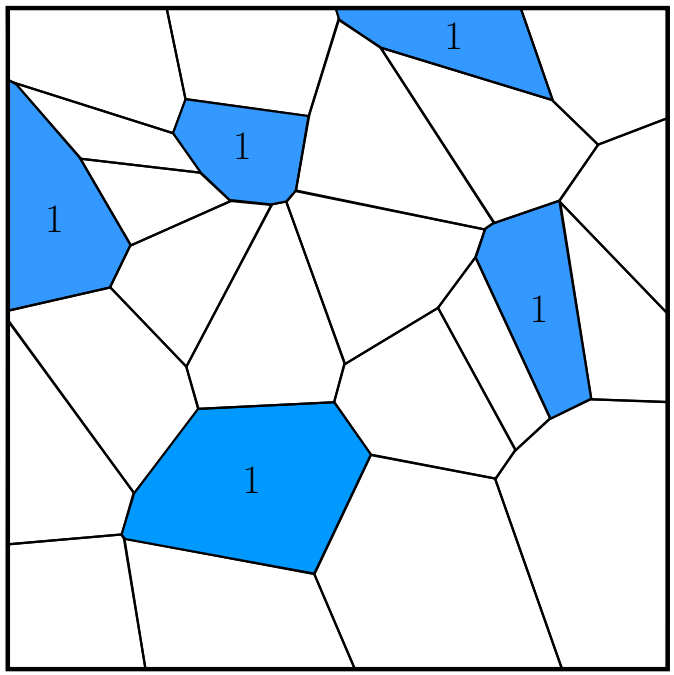

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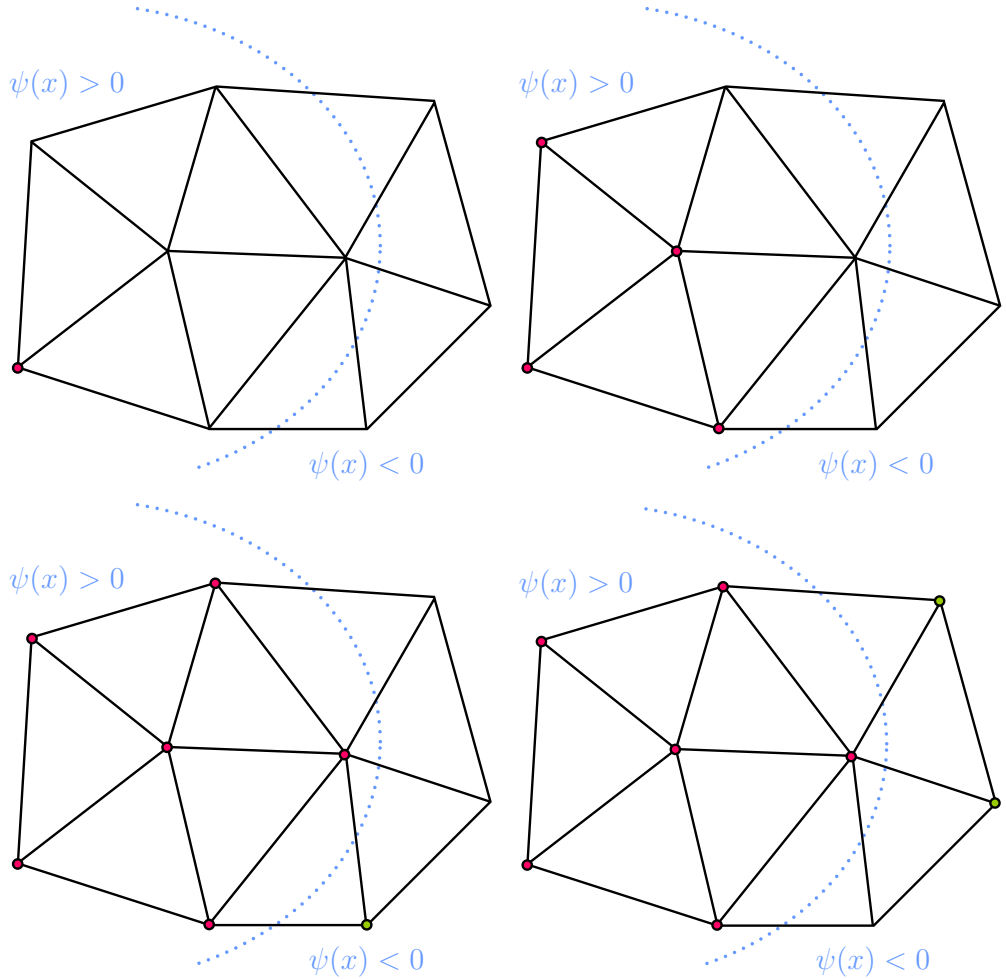

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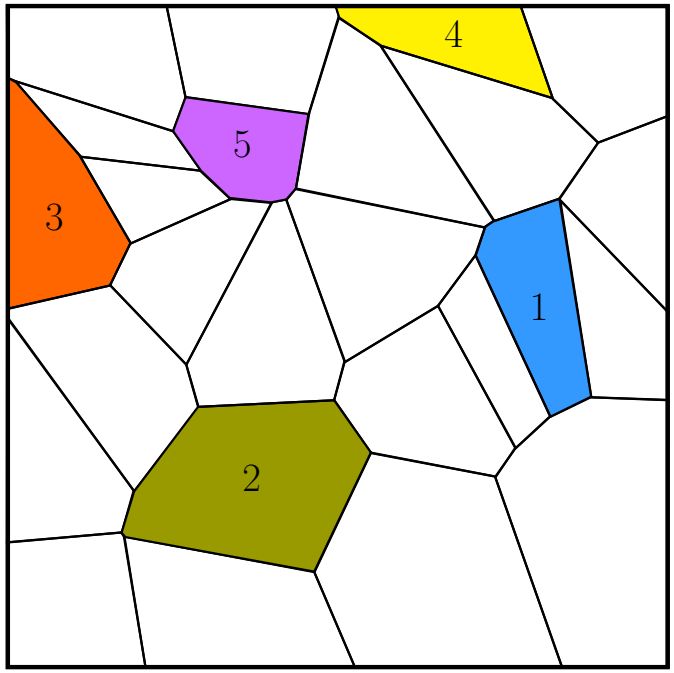
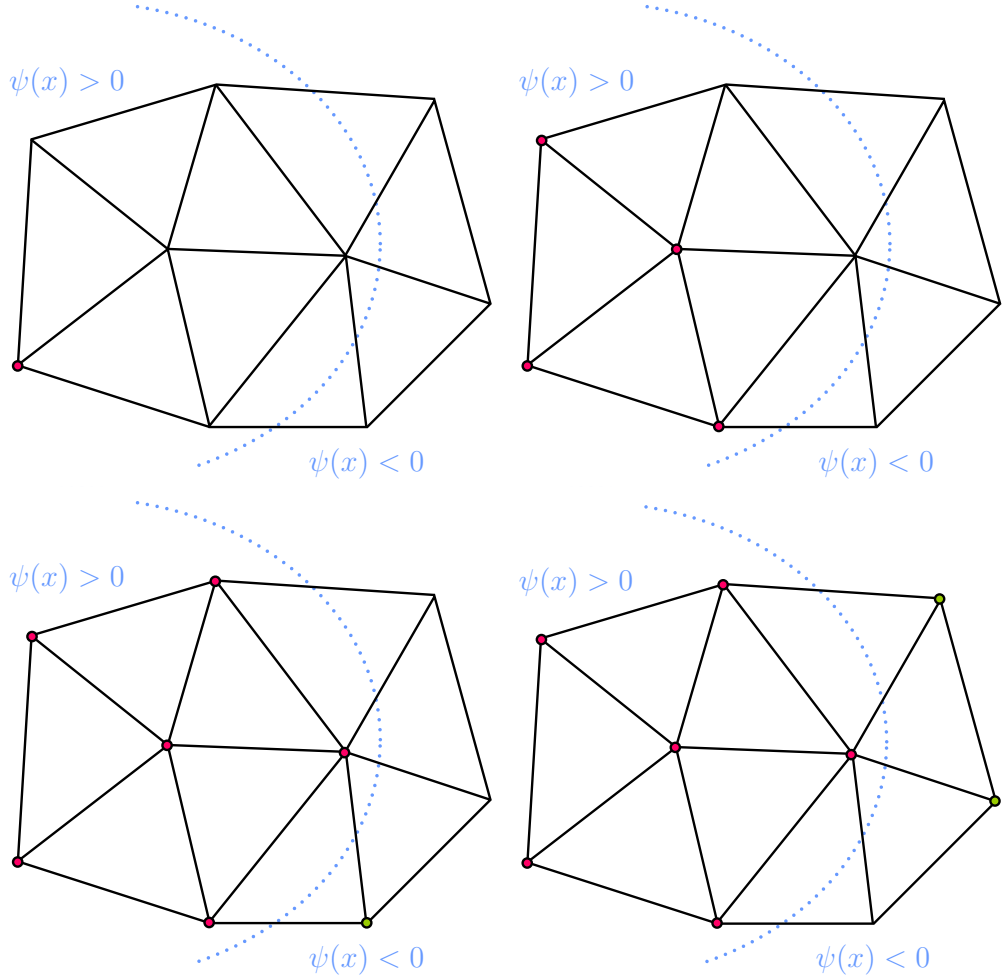


Index field obtained after performing the SCC procedure



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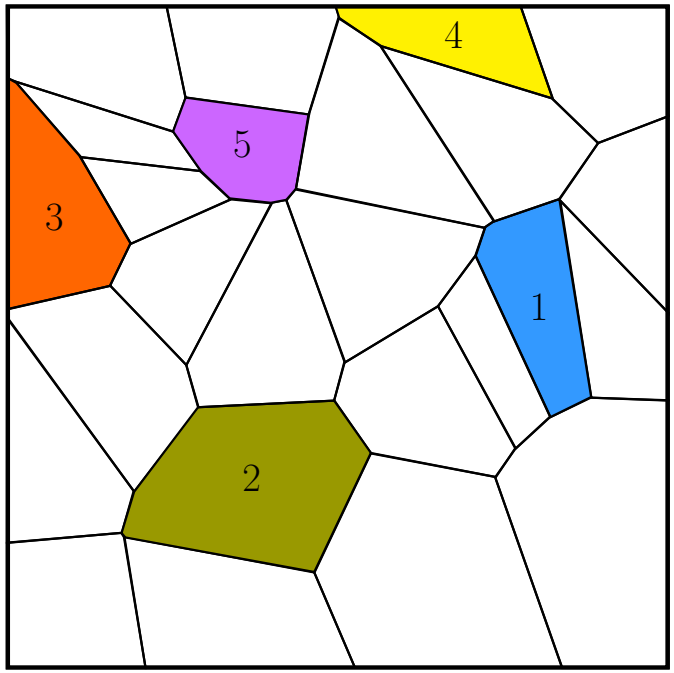

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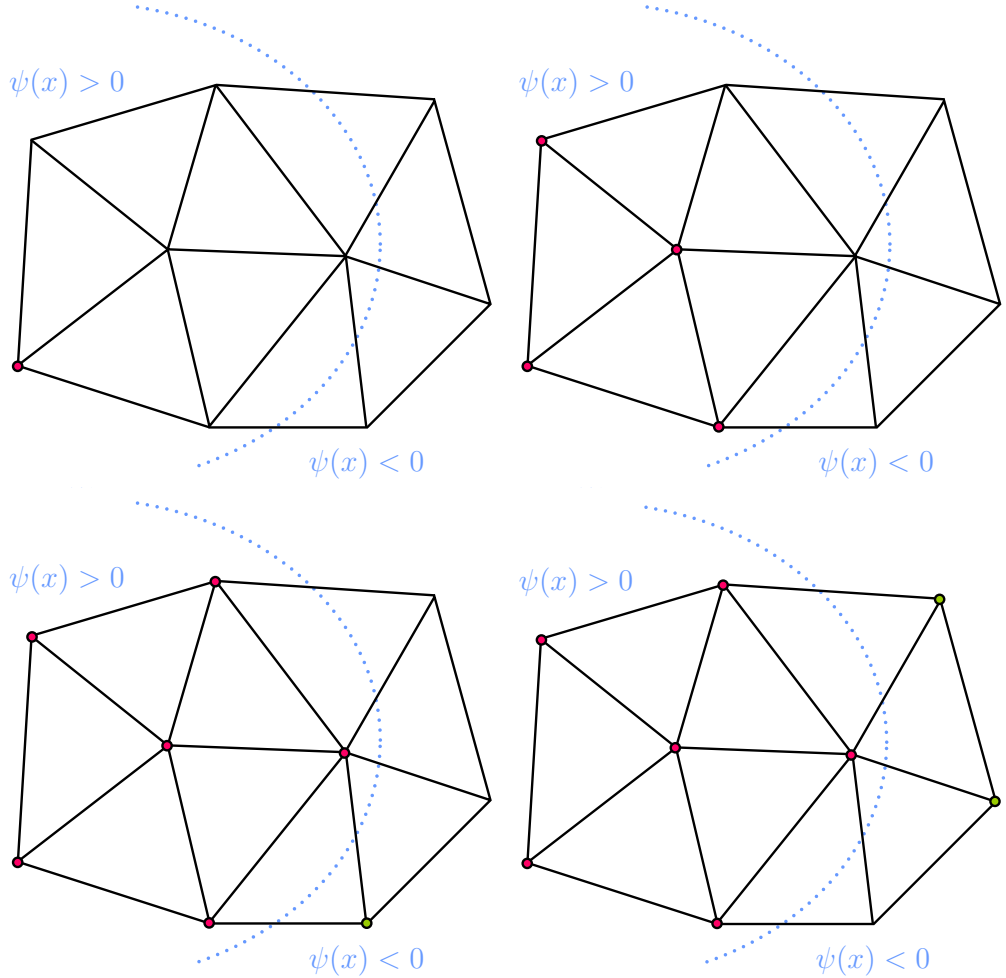
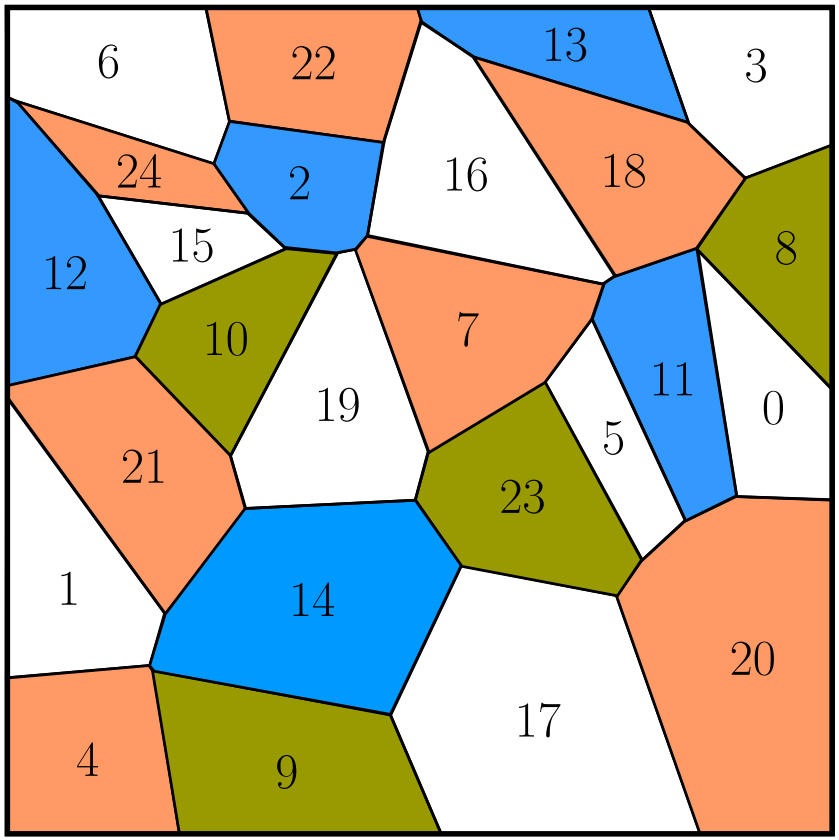


And... in parallel?

That's an other story... (see the publication below)

B. Scholtes, M. Shakoor, A. Settefrati, P.-O. Bouchard, N. Bozzolo, M. Bernacki "New finite element developments for the full field modeling of microstructural evolutions using the level set method" *Comp. Mat. Sci.* (2015)

Swapping algorithm



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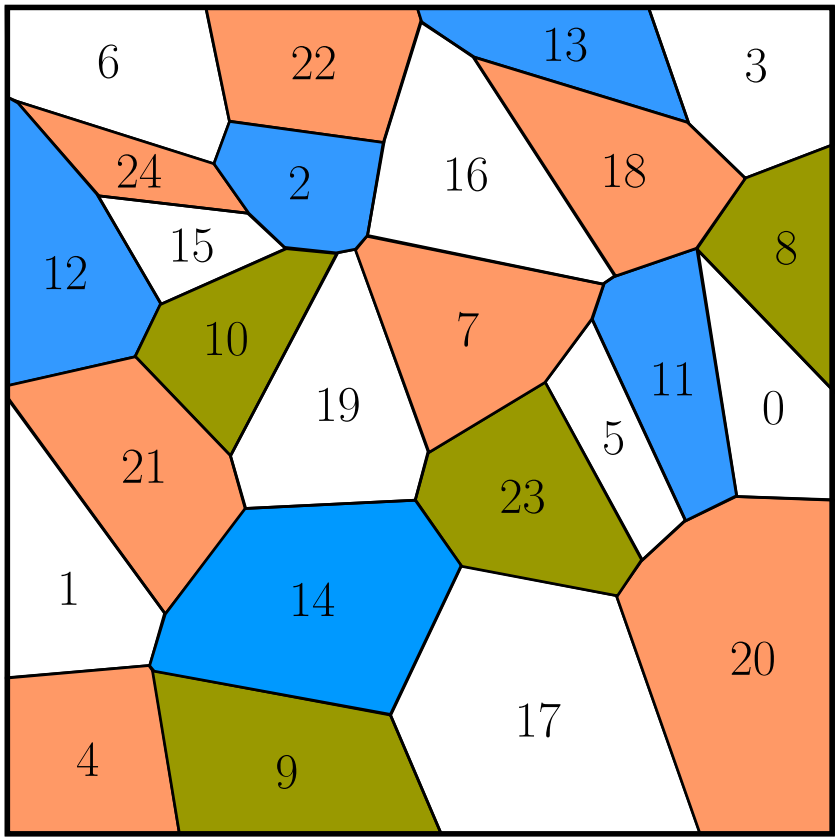

The recoloring procedure:

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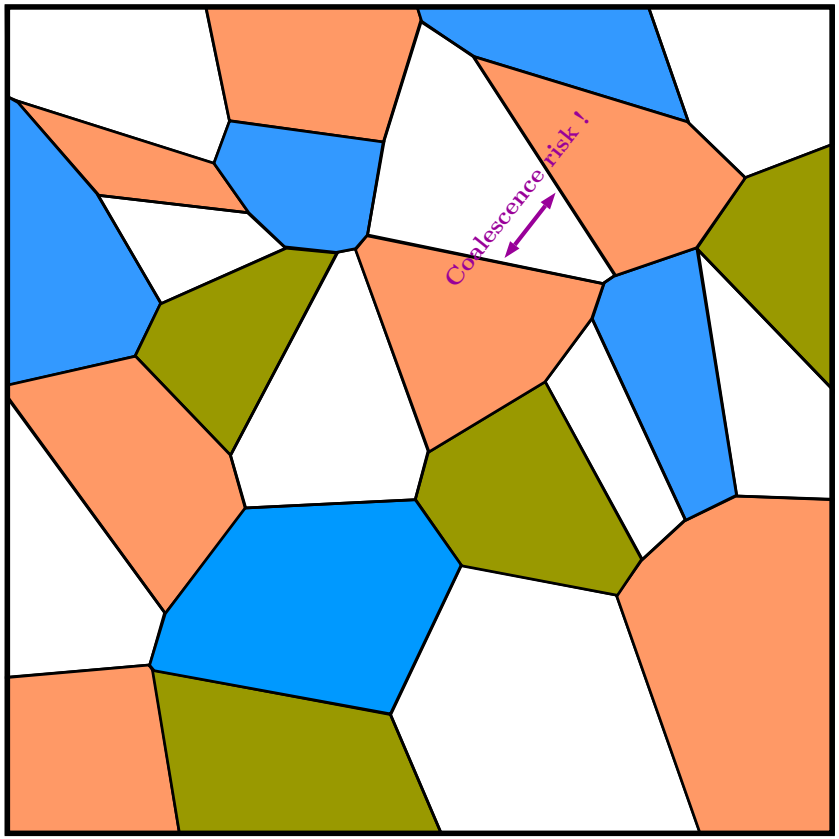

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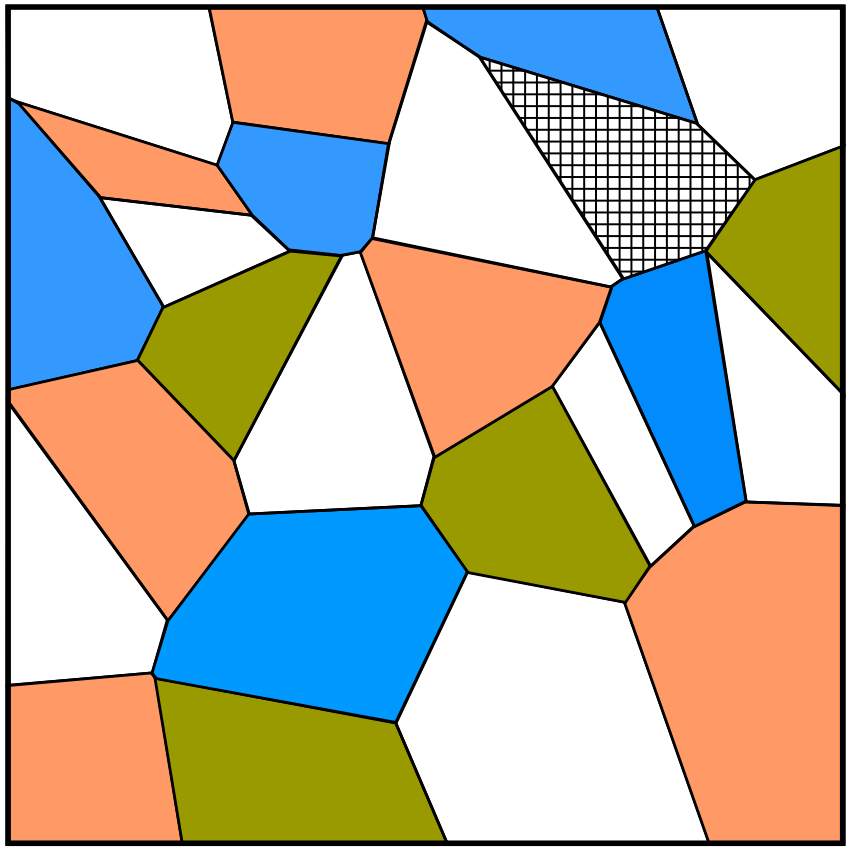

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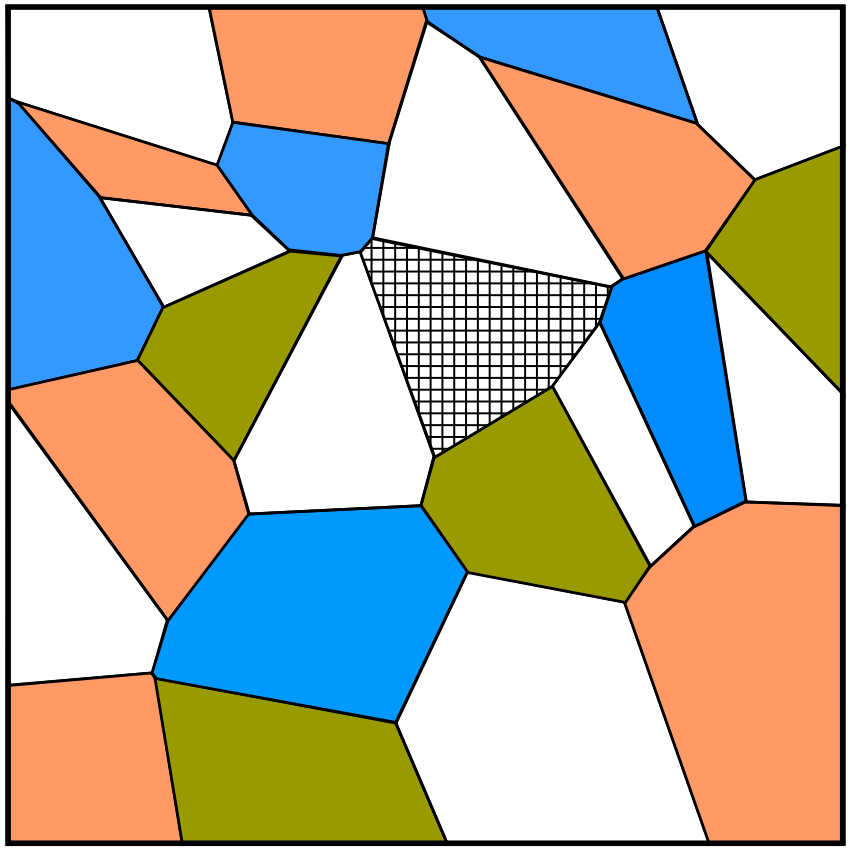

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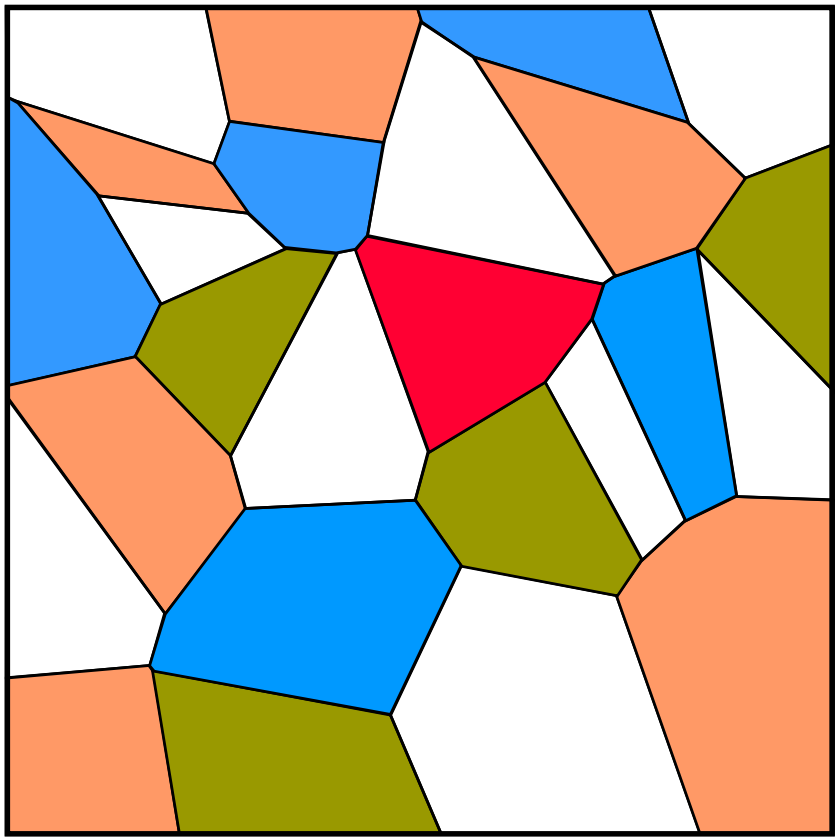

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2. Try to find another color (GLS function) for one of the grain, which could host this grain without generating a new conflict
3. If (2) failed, try with the other grain
4. If (2) and (3) failed, initialize a new GLS function and transfer one of the grain inside this GLS function

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Krill III et al. "Computer simulation of 3-D grain growth using a phase-field model" *Acta Mat.* (2002)

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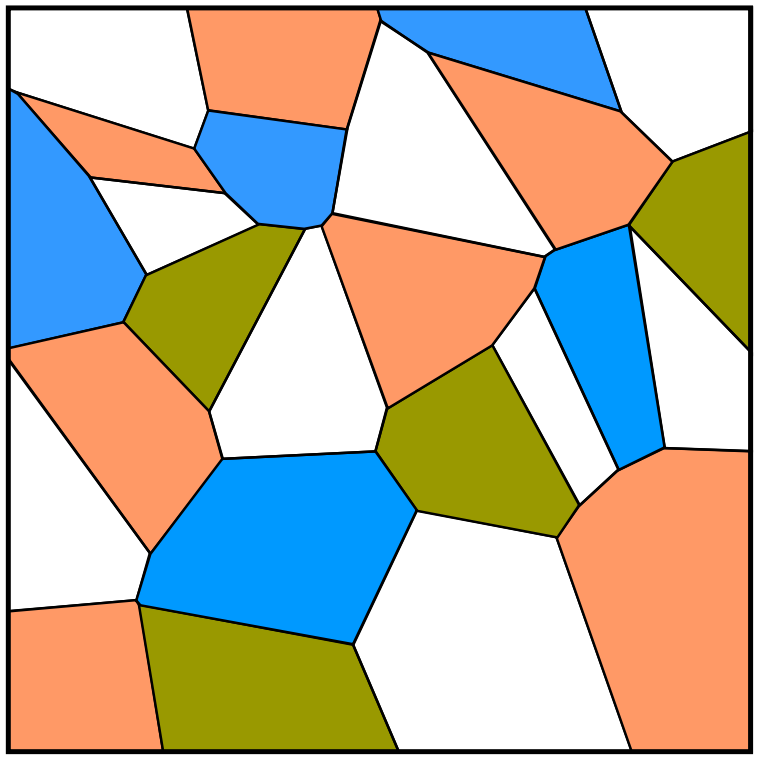
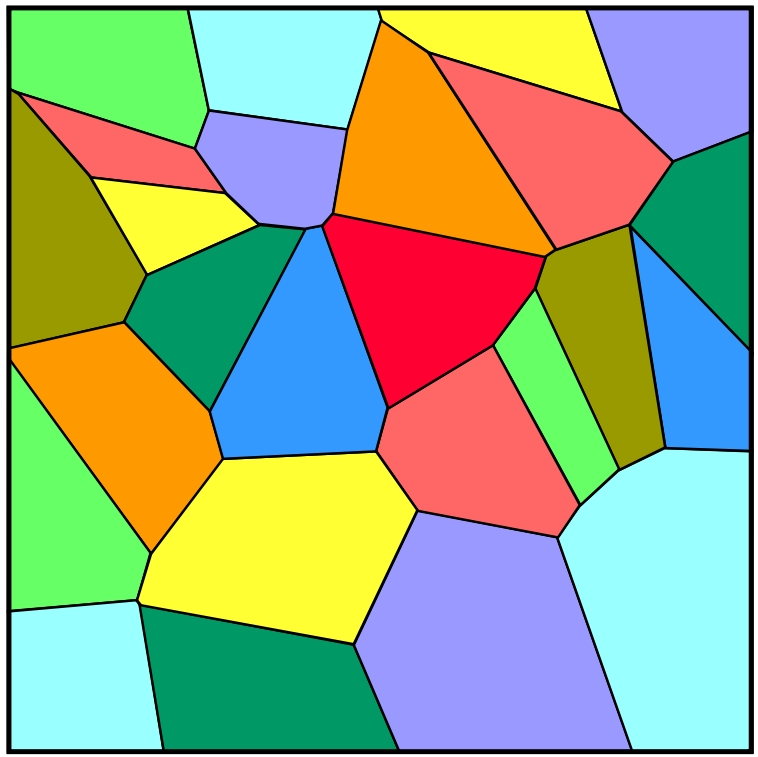
Coalescence

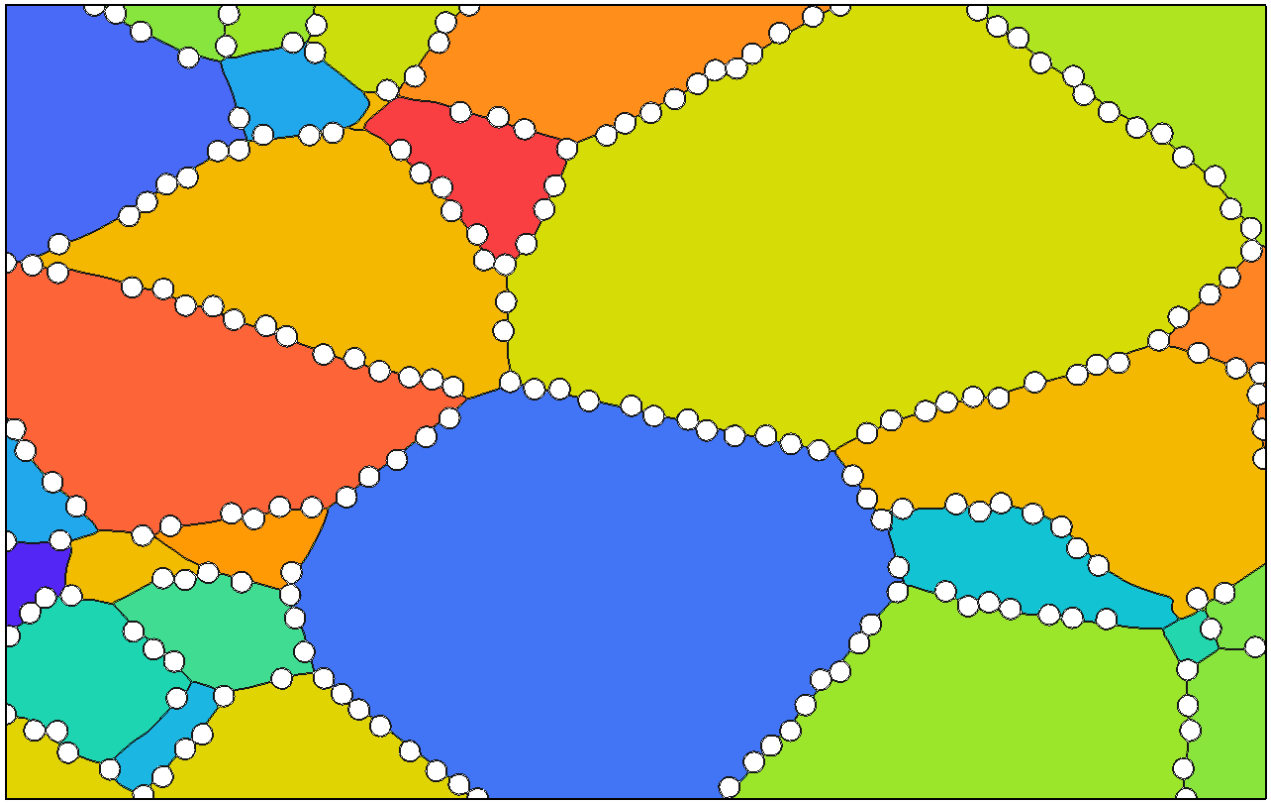


25 grains represented by 4 colors



After recoloring: 25 grains represented by 10 colors (with a minimal separation of two grains between a given color

Discussion of the swapping criterion

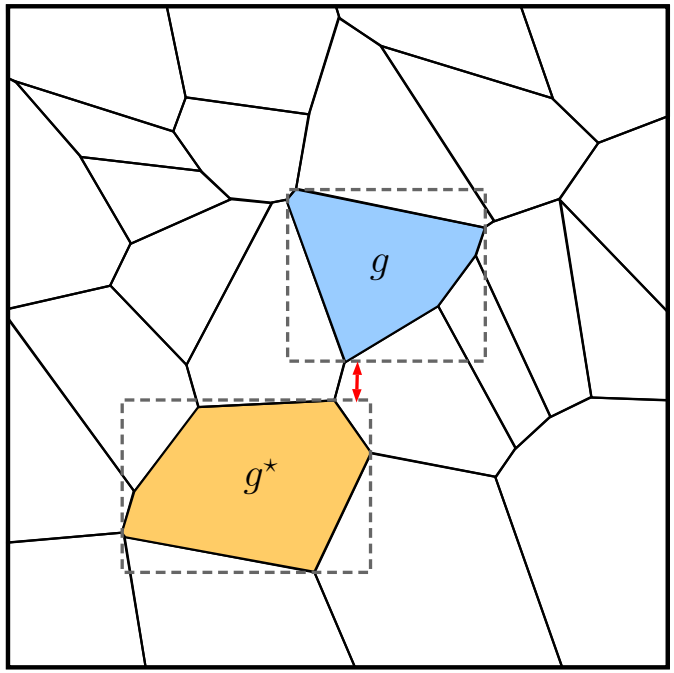


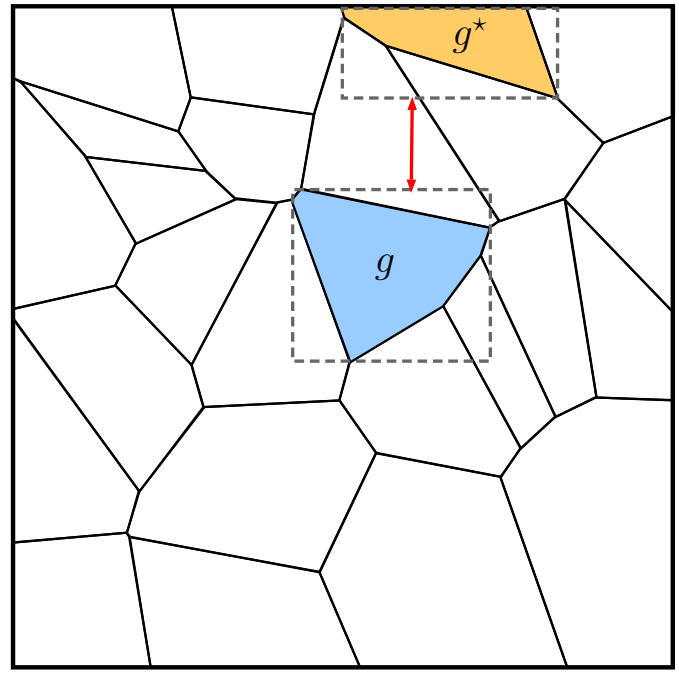
The distance between the grains is important too!

B. Scholtes, M. Shakoor, A. Settefrati, P.-O. Bouchard, N. Bozzolo, M. Bernacki "New finite element developments for the full field modeling of microstructural evolutions using the level set method", *Computational Materials Science* (2015)

B. Scholtes, R. Boulais-Sinou, A. Settefrati, D. Pino Munoz, I. Poitrault, A. Montouchet, N. Bozzolo, M. Bernacki "3D level set modeling of static recrystallization considering stored energy fields", *Computational Material Science (2016)*

Algorithm optimization: use of bounding boxes to evaluate coalescence risk





Redefinition of the long range neighborhood:

1. In order to limit the number of recoloring operations and then to reduce the number of created GLS functions
2. Concept: If $g^\star$ a second neighbor of g is *relatively* far from g, it can be safely ignored when creating the table $\mathcal{L}(g)$

B. Scholtes, M. Shakoor, A. Settefrati, P.-O. Bouchard, N. Bozzolo, M. Bernacki "New finite element developments for the full field modeling of microstructural evolutions using the level set method", *Computational Materials Science* (2015)

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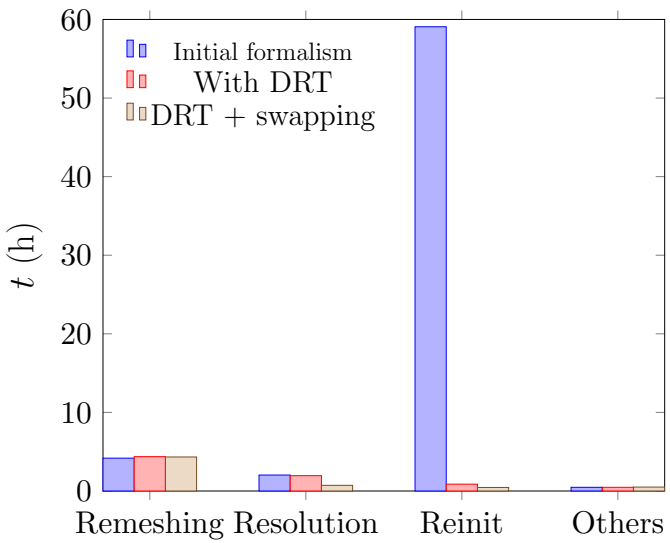

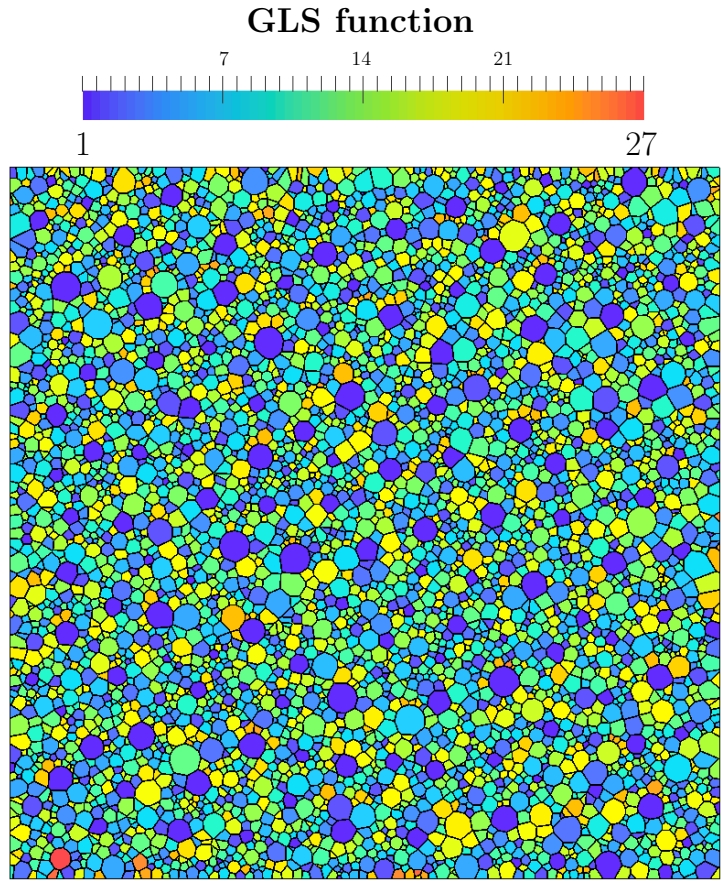

Initial 2D polycrystal (5000 grains)

With DRT + swapping: acceleration factor → 11 + coalescence avoided in any situation!

Improvement of simulation time for 3D simulation

A simple grain growth case (12 CPUs)

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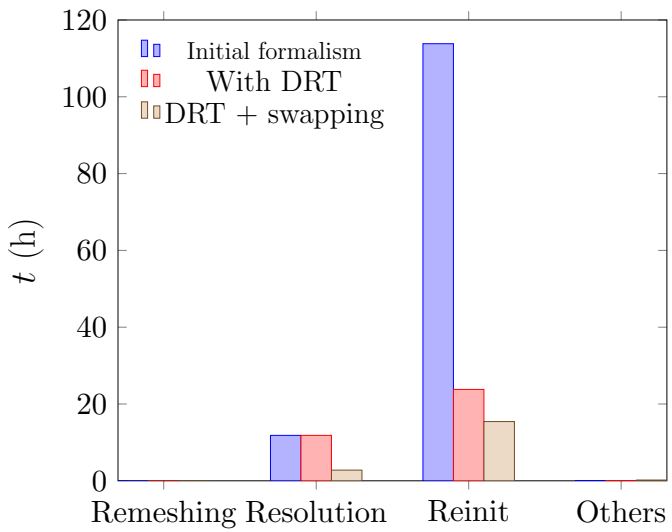
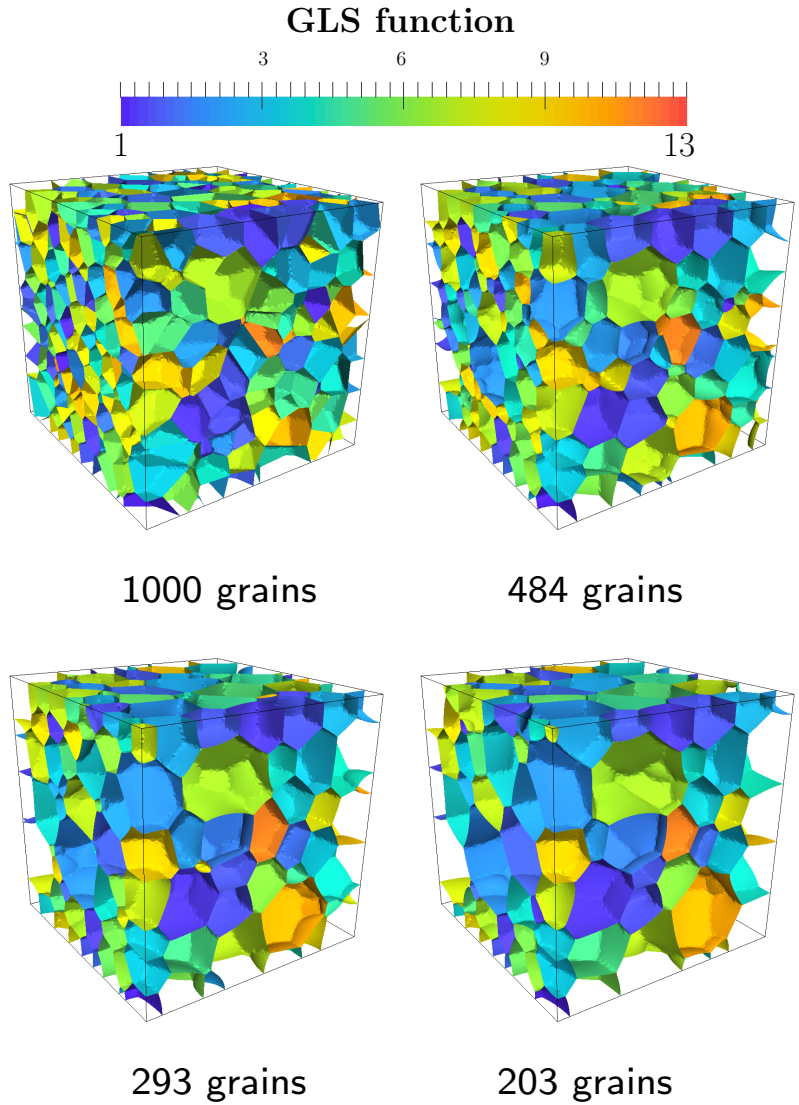




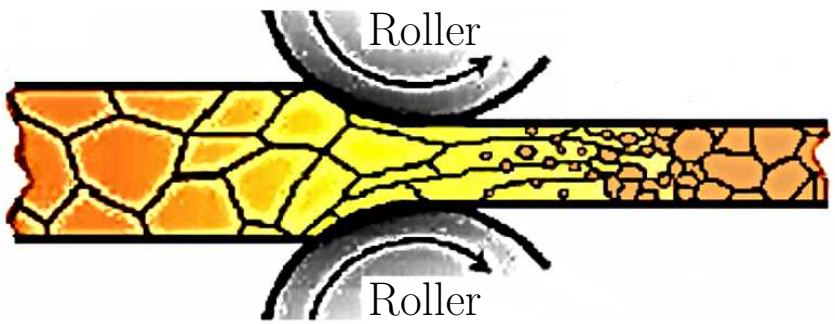
With DRT + swapping: acceleration factor → 7
+ coalescence avoided in any situation!

Outline

Outline

What is static recrystallization (SRX) ?

- Migration of the grain boundary under combined effects of stored energy gradients and interface curvature
- Initiated after the deformation stage
- Nuclei (grains free of dislocations) may appear during SRX or only at the early stage (site-saturated nucleation)

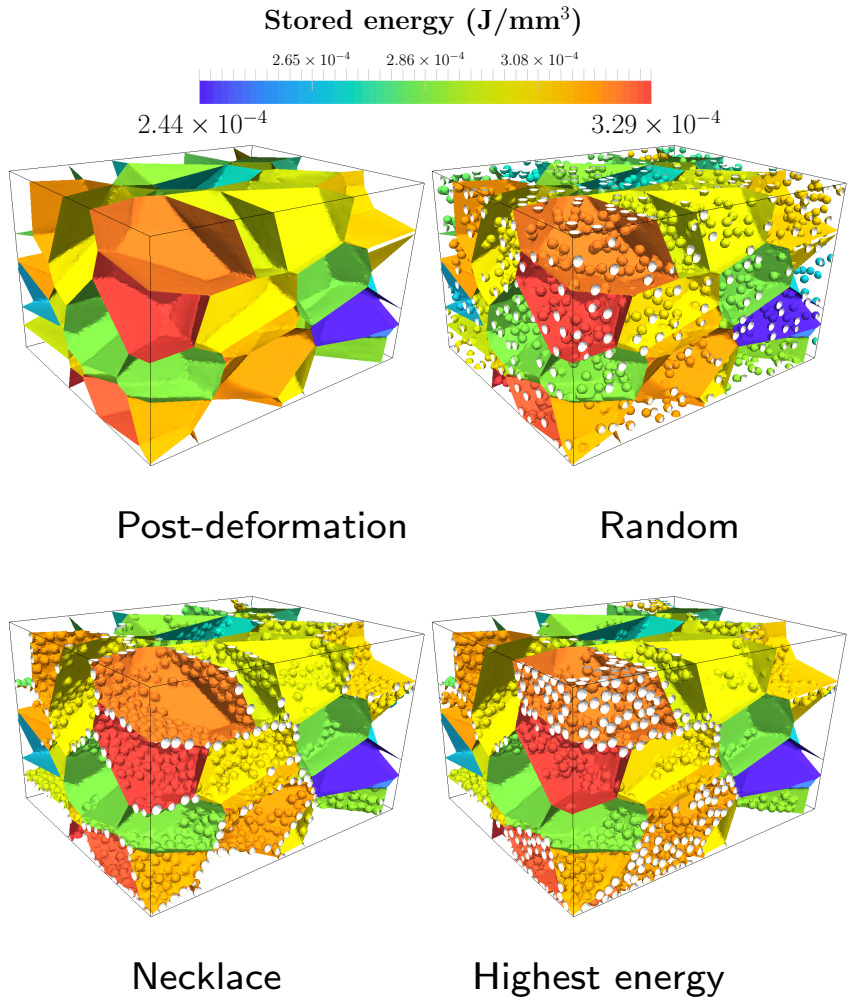


$$\begin{cases} \dfrac{\partial \psi}{\partial t} - M\gamma\Delta\psi + \vec{v}^{e}\nabla\psi = 0 \\ \psi(x, t=0) = \psi^{0}(x) \end{cases}$$

SRX simulation of a 304L austenitic steel

Configuration

- 1/4h of heat treatment at 1000°C
- Initial polycrystal composed of 100 grains + 3000 nuclei
- Material : 304L austenitic steel
- Applications : ArcelorMittal AREVA



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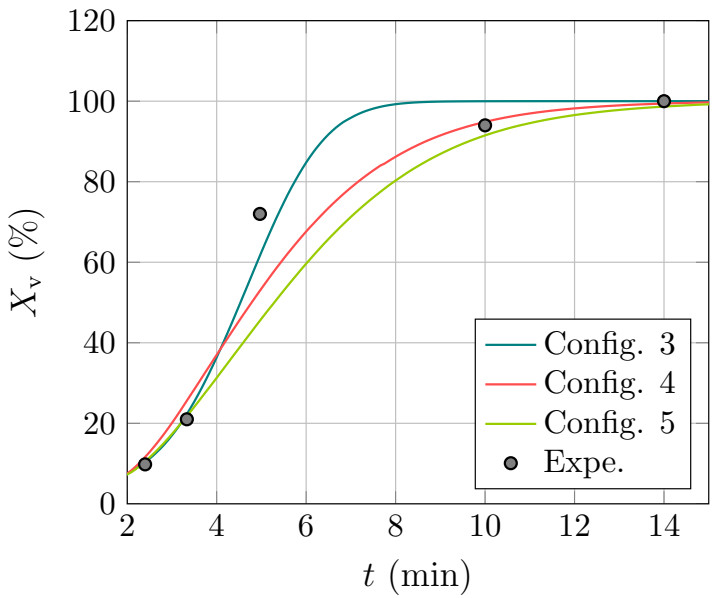

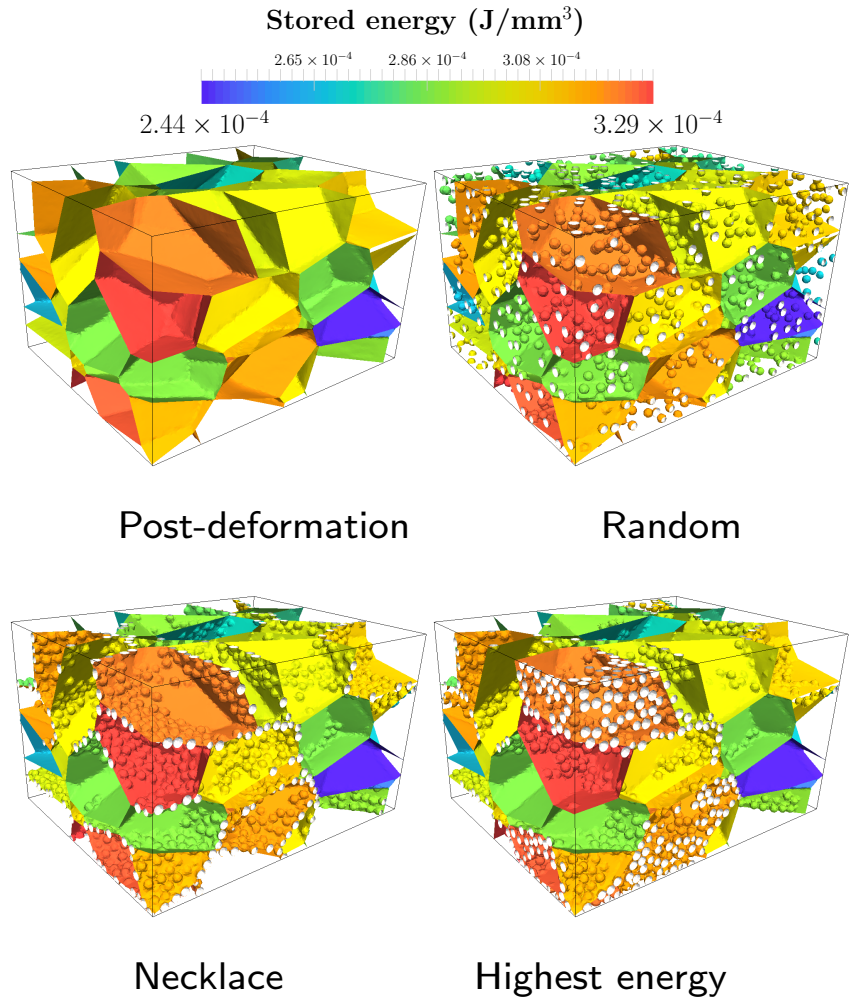

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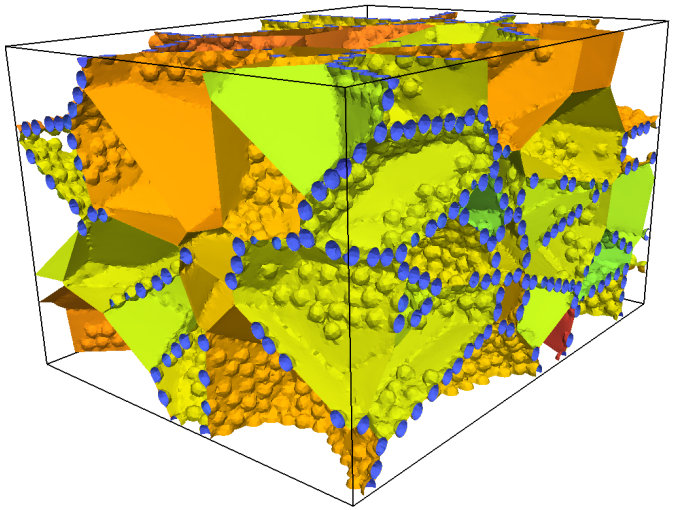
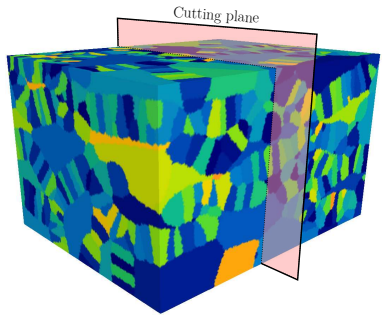
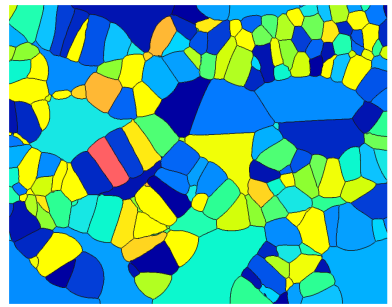
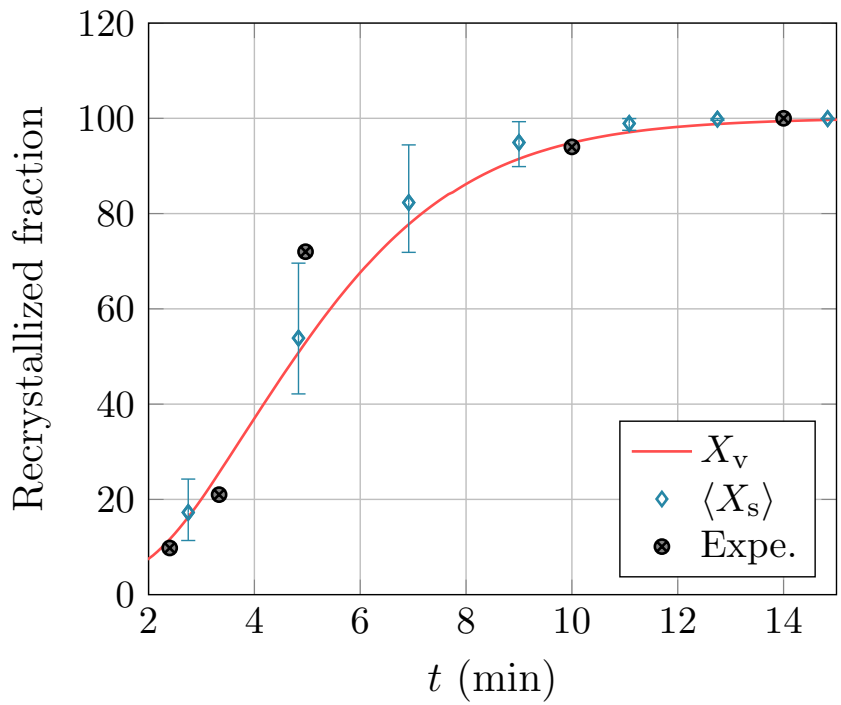
SRX simulation of a 304L austenitic steel



3D simulation of SRX in 304L

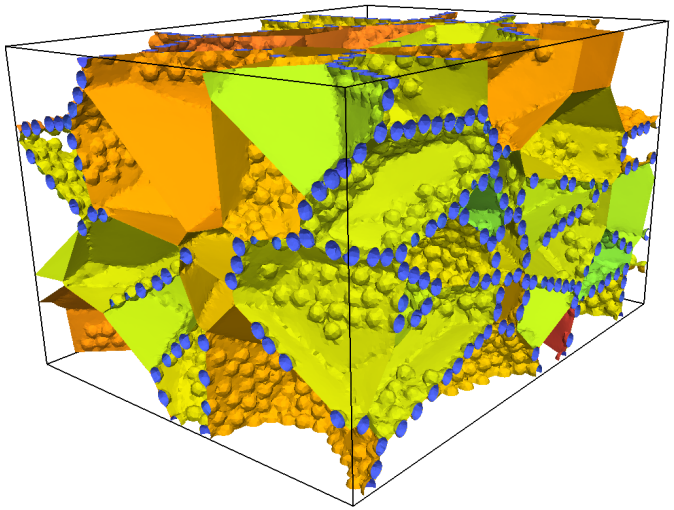




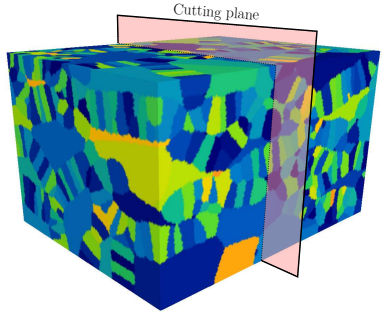


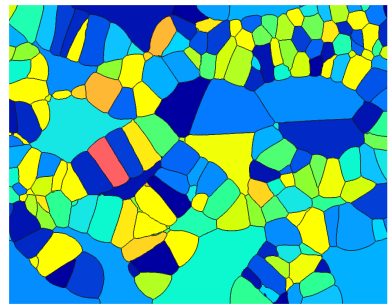
B. Scholtes, R. Boulais-Sinou, A. Settefrati, D. Pino Munoz, I. Poitrault, A. Montouchet, N. Bozzolo, M. Bernacki "3D level set modeling of static recrystallization considering stored energy fields", *Computational Material Science (2016)*

SRX simulation of a 304L austenitic steel



3D simulation of SRX in 304L

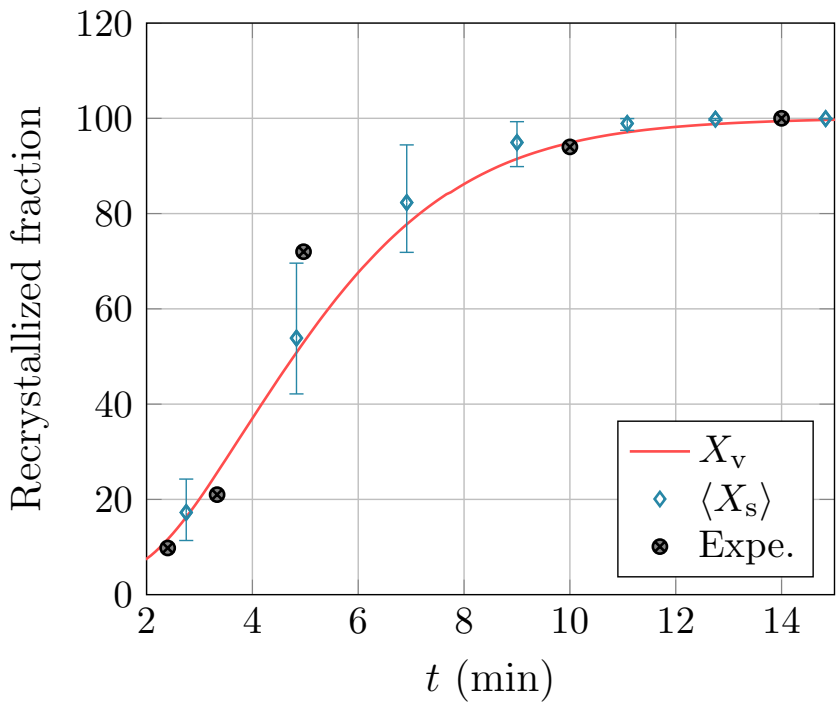




Obtained simulation times

- Around 24h with the new formalism (Scholtes et al. 2016)
- Estimated around 1 month 20 days at the beginning of this thesis work

Estimated acceleration factor $\rightarrow$ 45



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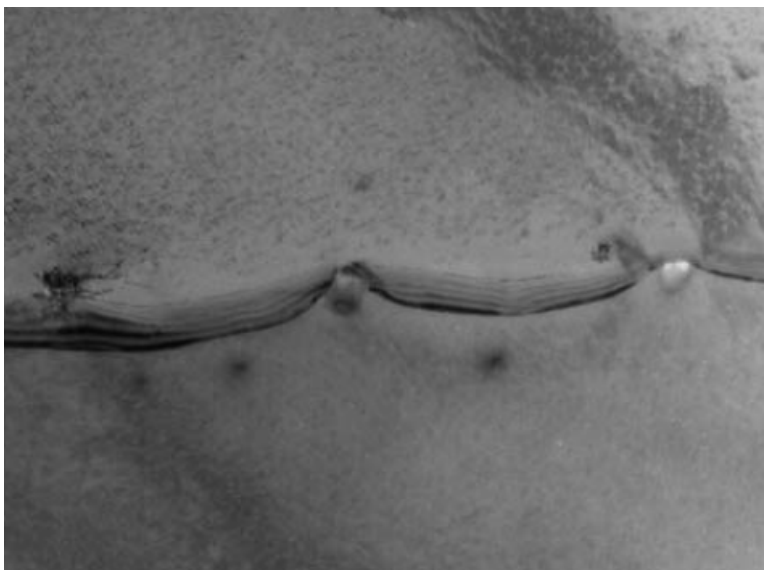
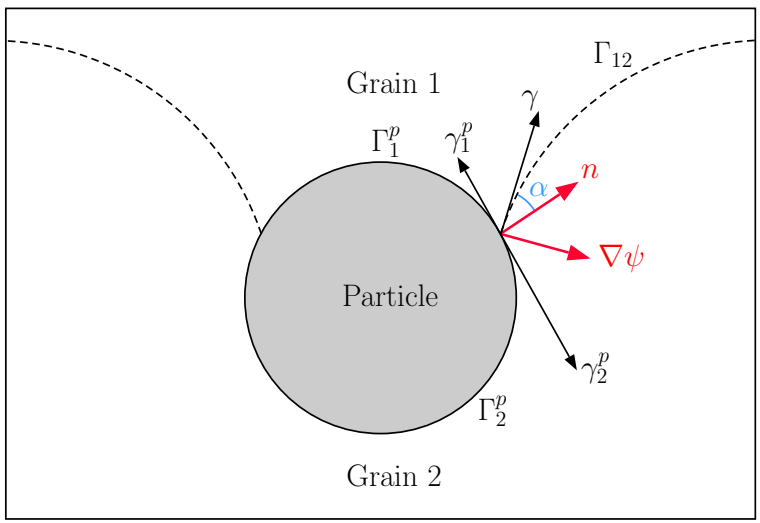
Outline

Zener pinning in superalloys

- Addition of a low-solubility element which precipitates as second phase particles (SPP)
- Particles hinder the migration of grain boundaries
- This phenomenon is used to control the grain size growth





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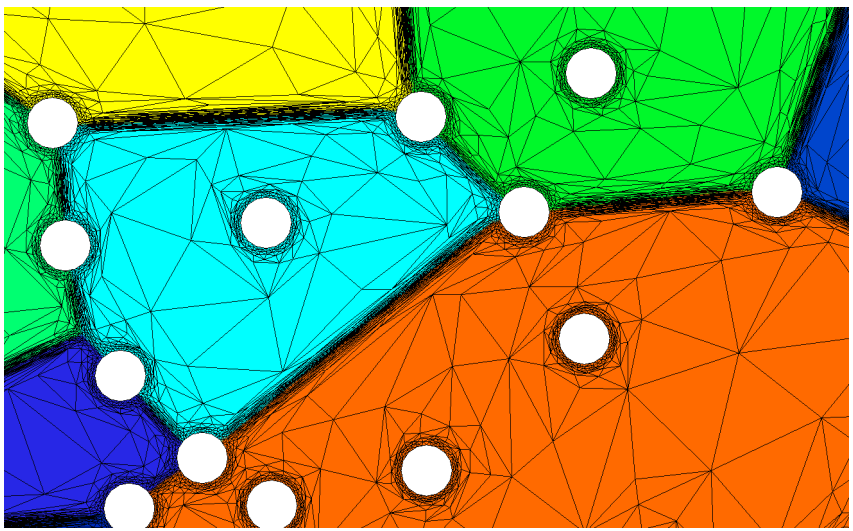


$$\begin{cases} \dfrac{\partial \psi}{\partial t} - M\gamma\Delta\psi = 0 \\ \psi(x, t=0) = \psi^0(x) \end{cases}$$

Classical mean field models

$$\langle R_f \rangle = A \frac{r_p}{f_v^b} \qquad \langle R_f \rangle = K \frac{r_p}{f_{gb}^m}$$

- $\langle R_f \rangle$: mean grain size at steady state
- f_v : particle volume fraction
- f_{gb} : volume fraction of particles located at the GB in the frozen microstructure
- r_p : mean particle radius
- A, K, b, m : fitting parameters $\rightarrow$ a lot of values proposed in the literature

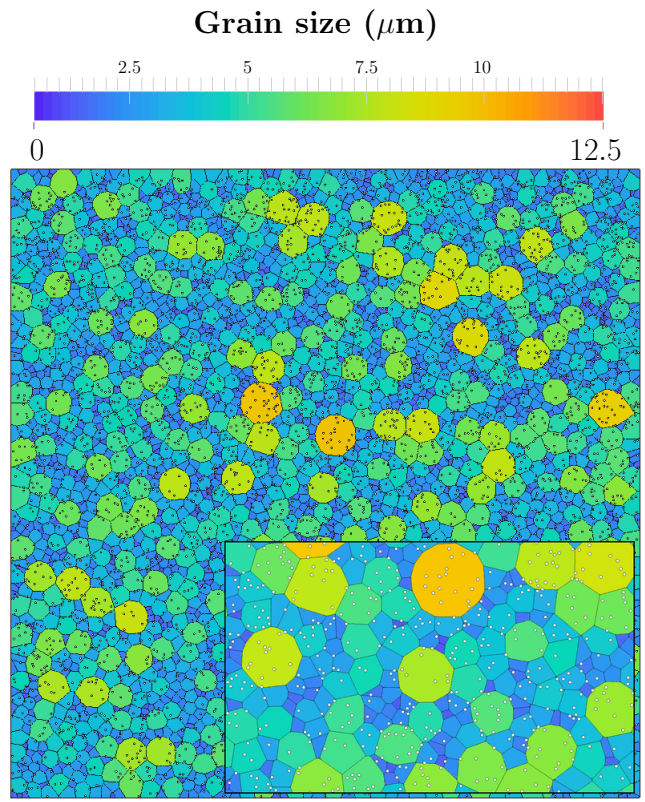
---

Manoar et al. "Five decades of the Zener equation" *ISIJ International* (1998)

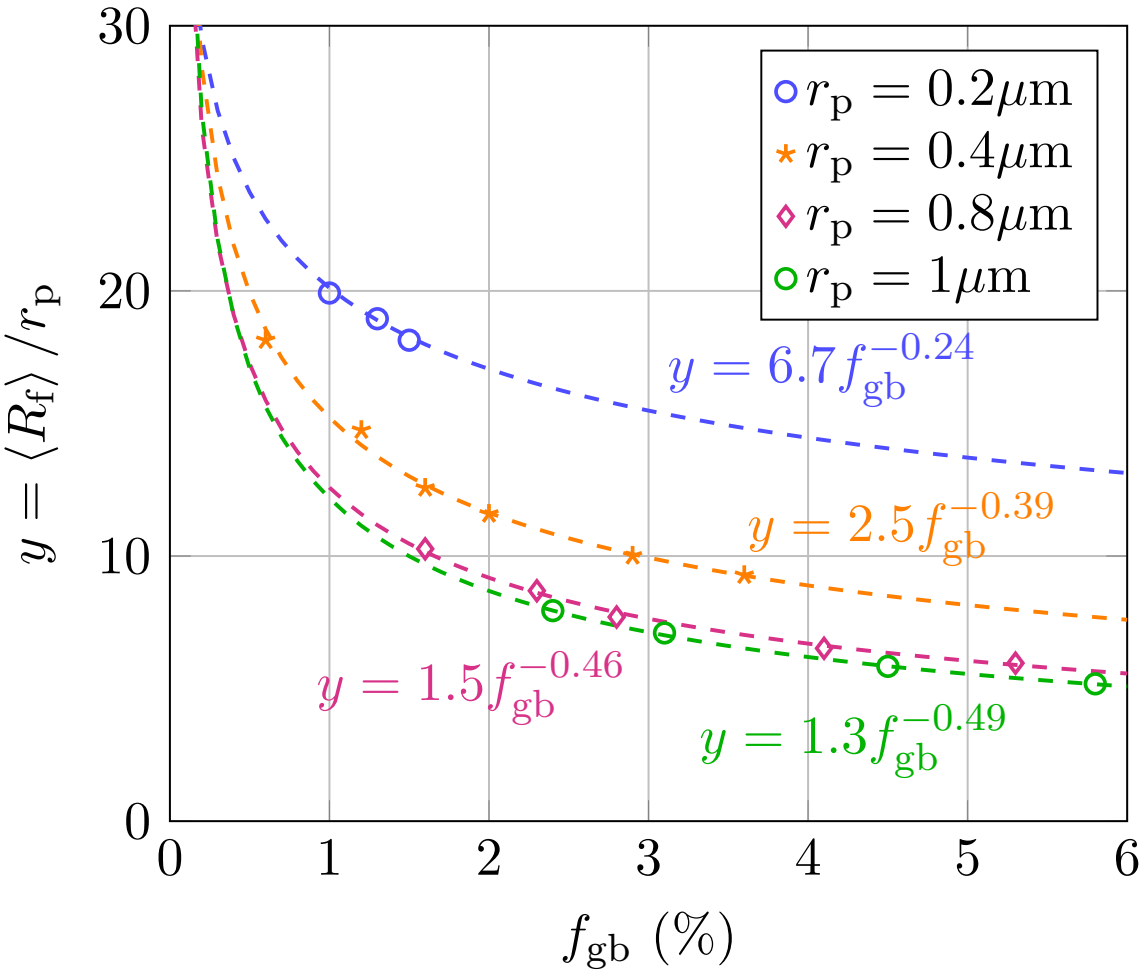
Moelans et al. "Phase field simulations of grain growth in two-dimensional systems containing finely dispersed second-phase particles" *Acta Mat.* (2006)

Full field experiments

- Material : Inconel 718 (initial mean grain size $\langle R_0 \rangle = 3.5\mu$m)
- 2600 grains in the initial microstructure
- 4 particle radii investigated : $r_p = 0.2\mu$m, 0.4μm, 0.8μm, 1μm
- $2\% < f_v < 10\%$
- At steady state, we measure the $\langle R_f \rangle$ and f_{gb}
- Between 1 and 3 days of computations using up to 16 CPUs for the simulations



Results of full field simulations



Results of 2D pinning simulations for Inconel 718 with different particle volume fractions and radiuses. Each point is the result of a full field simulation.

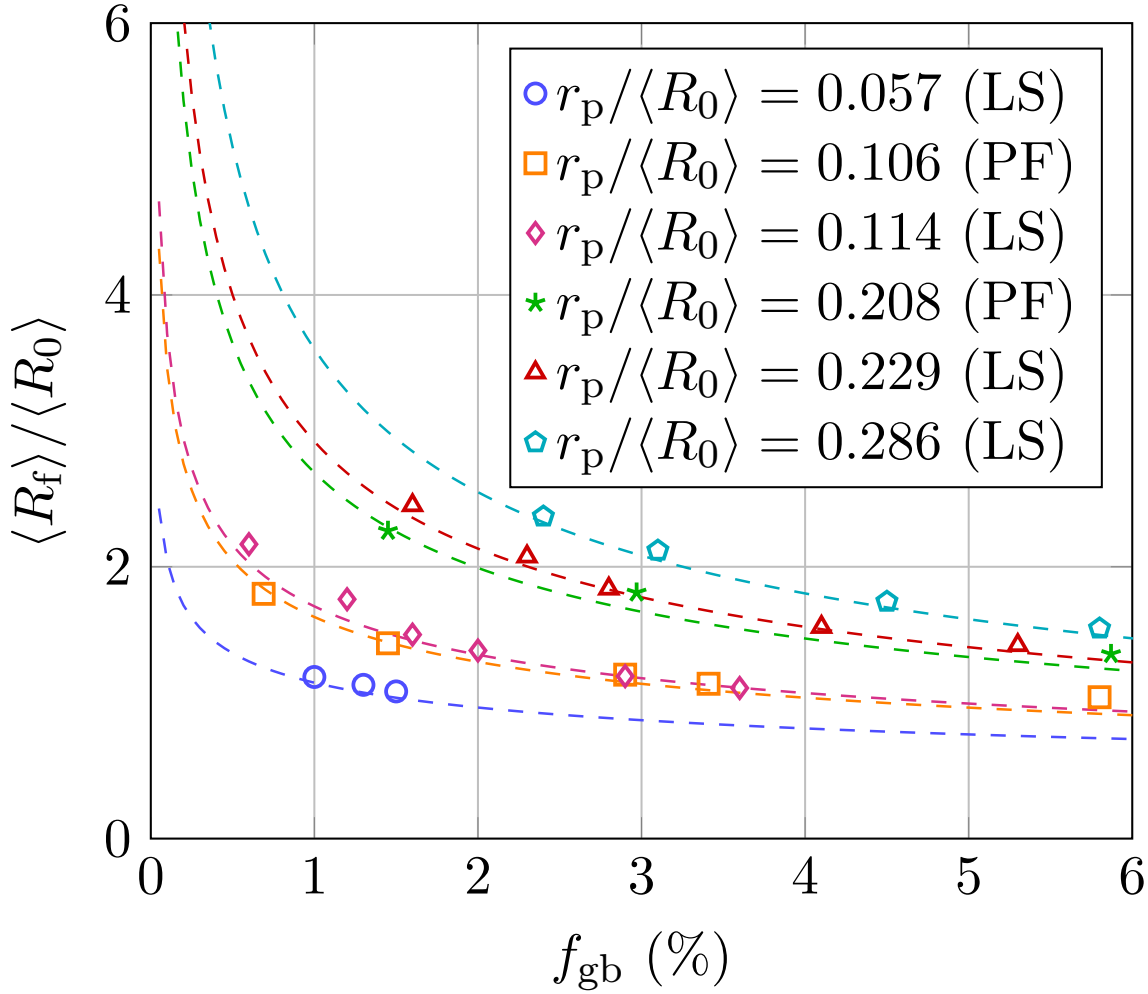
2D pinning simulations: summary

- In the modified Zener law, the parameter K and m are generally assumed constant
- This study has demonstrated they actually depend on the particle radius r_p
- This result may explain the versatility of the values reported in the literature for these parameters
- Based on the full field simulation results, a new form is proposed for the limiting mean grain size equation:

$$\langle R_f \rangle = 0.362 \cdot \langle R_0 \rangle \cdot f_{gb}^{-0.853 \left(\frac{r_p}{\langle R_0 \rangle} \right)^{0.428}}$$

B. Scholtes, D. Ilin, A. Settefrati, N. Bozzolo, A. Agnoli, M. Bernacki "Full field modeling of the Zener pinning phenomenon in a level set framework - discussion of classical limiting mean grain size equation" *Superalloys 2016: 13th International Symposium on Superalloys* (2016)

Model validation



Prediction of the newly proposed mean field model (dash lines) for different SPP/grain size ratio and comparison with the results of full field simulations (PF simulation from (Moelans et al. 2006) and LS-FE simulations).

Moelans et al. "Phase field simulations of grain growth in two-dimensional systems containing finely dispersed second-phase particles" *Acta Mat.* (2006)

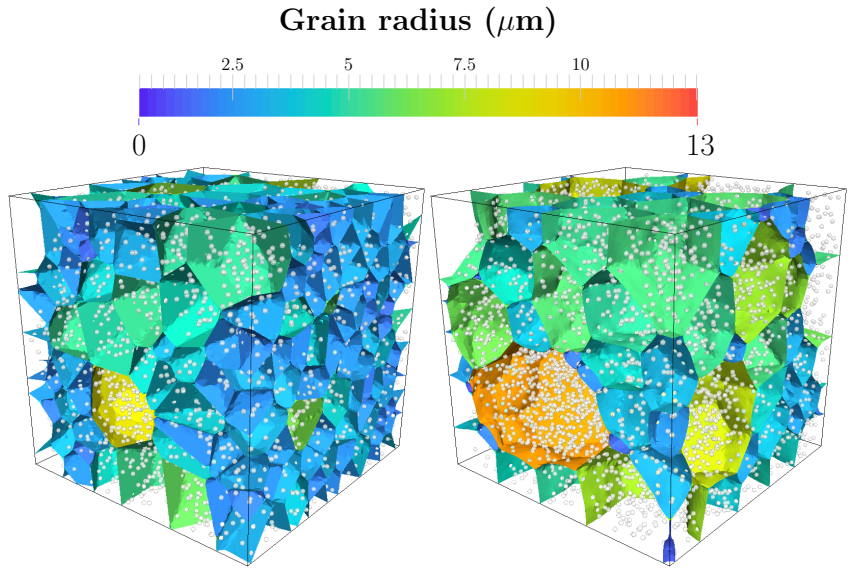
First realistic 3D LS/FE simulation of Zener pinning

Configuration

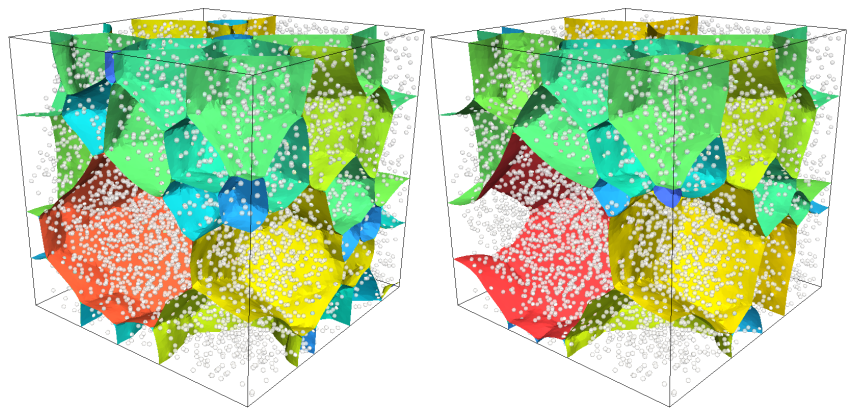
- 4min of heat treatment at 950°C
- Initial polycrystal composed of 530 grains
- Material : Inconel 718
- $r_p = 0.35\mu$m, $f_v = 2\%$ (10000 particles)
- Applications : SAFRAN AEROSPACE · DEFENCE · SECURITY AUBERT&DUVAL

Simulation time

- 2 days and 10 hours using 24 CPUs
  $\rightarrow$ outstanding compared with the state of the art



530 grains 138 grains



75 grains 54 grains

Outline

Conclusions

- Significant improvement of the numerical efficiency $\rightarrow$ acceleration factors ≈ 45 for realistic SRX applications
- We are now able to tackle 3D simulations of GG, SRX and Zener pinning with very interesting computation times
- Completely generic numerical tools $\rightarrow$ many applications (solidification, additive manufacturing, powder compaction, ductile damage mechanisms,...)
- The developments have been integrated in the commercial software DIGIMU®
- 5 publications in international journals + 5 conference proceedings
- 11 international oral communications + participation in 10 national workshops

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Nguyen "Multiscale finite element modeling of macrosegregation and grain transport", *PhD MINES ParisTech (2015)*

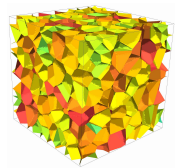
Saad "Numerical modelling of macrosegregation formed during solidification with shrinkage using a Level Set approach", *PhD MINES ParisTech (2016)*

Chen et al. "Finite element modeling of deposition of ceramic material during SLM additive manufacturing", *Proceedings of Numiform 2016 (2016)*

Trejo et al. "Ductile fracture - influence of an heterogeneous microstructure on nucleation, growth and coalescence mechanisms", *Proceedings of Numiform 2016 (2016)*

Prospects

Metallurgical aspect:

- Anisotropy, collaboration with Ulm university (PhD J. Fausty 2016-2019, Chair OPALE)
- Phase transformation (Upcoming PhD, Chair DIGIMU)
- Experimental/numerical confrontations (Collaboration N. Bozzolo, Team MSR)
- Dynamic recrystallization (PhD L. Maire 2015-2018) 

L. Maire et al. "Improvement of 3-D mean field models for capillarity driven grain growth based on full field simulations", *Journal of Materials Science (2016)*

Prospects

Numerical aspect:

- Management of the time step $\rightarrow$ has been largely initiated during this work (see manuscript)
- Simulation of dissolving SPP $\rightarrow$ first approach proposed in the manuscript (Upcoming PhD, Chair DIGIMU)
- Remeshing in 3D (Upcoming PhD, Chair DIGIMU)
- Handling of heterogeneous energy fields (Postdoctoral work of D. Ilin, Chair OPALE)
- Improvement of CPFEM code (Upcoming PhD, Chair DIGIMU)

"Merci!"

3.18 years

27,889 hours

100,400,400 seconds

In parallel...

A first simple approach

- Broadcast the full contour on each process, and build the full k-d tree on each process (redundant operation)
- The method remains competitive compared to classical approaches, but no speed-up in parallel

Recovering optimal efficiency

- Build a local contour and a local k-d tree on each process (independent operation)
- Compute local bounding boxes to each k-d tree and broadcast only the boxes
- Based on the boxes, interrogate other processors only when required

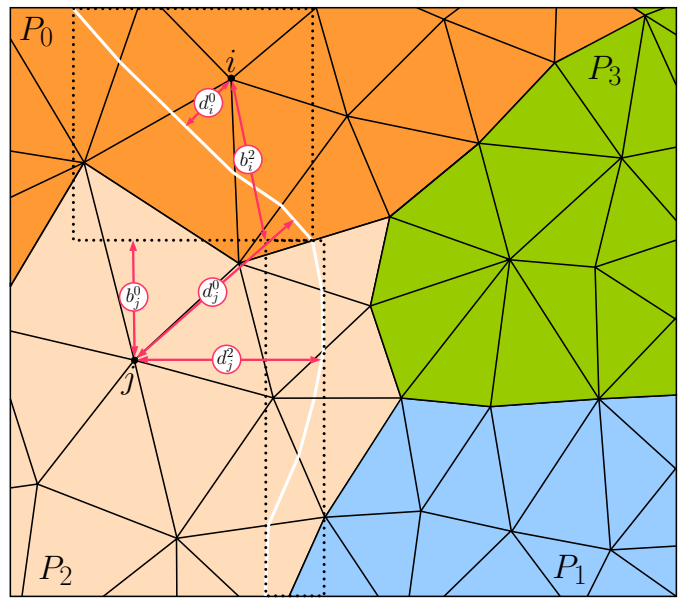
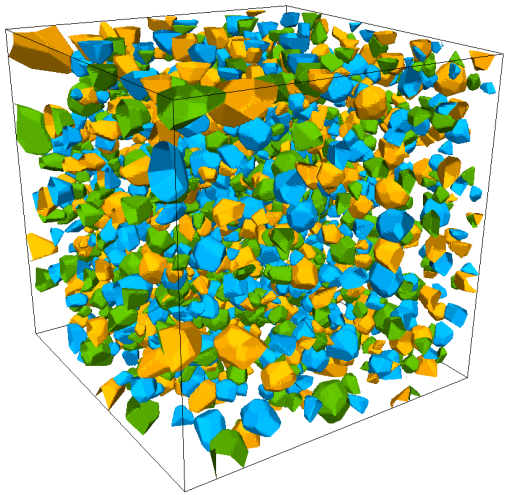


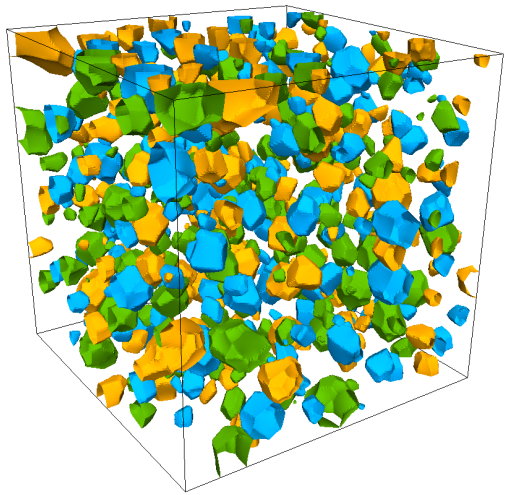
Illustration of the bounding box strategy used for parallel computations

M. Shakoor, B. Scholtes, P.-O. Bouchard, M. Bernacki "An efficient and parallel level set reinitialization method - Application to micromechanics and microstructural evolutions" *Accepted in Appl. Math. Model.* (2015)

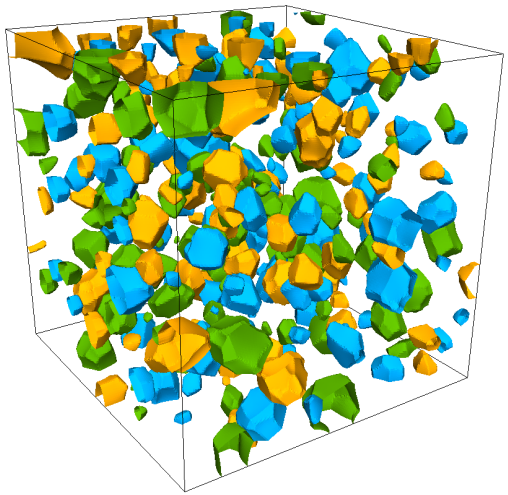
Large scale simulations and comparison with mean field approximations



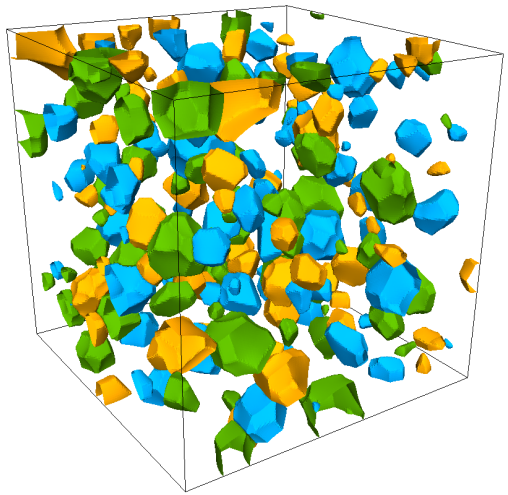
$t = 0$ (10000 grains)



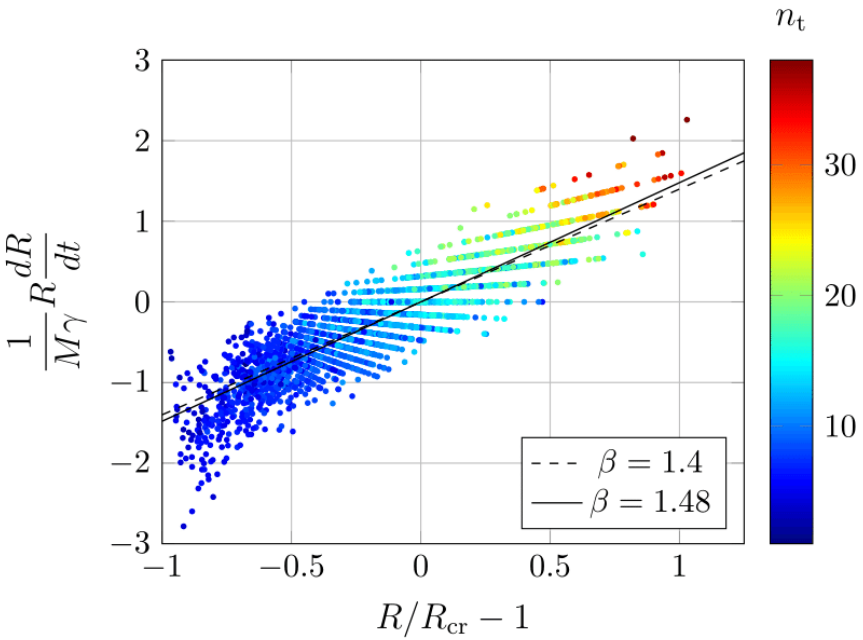
$t = 1/2t_h$ (4600 grains)



$t = 0$ (2750 grains)



$t = 1/2t_h$ (1950 grains)



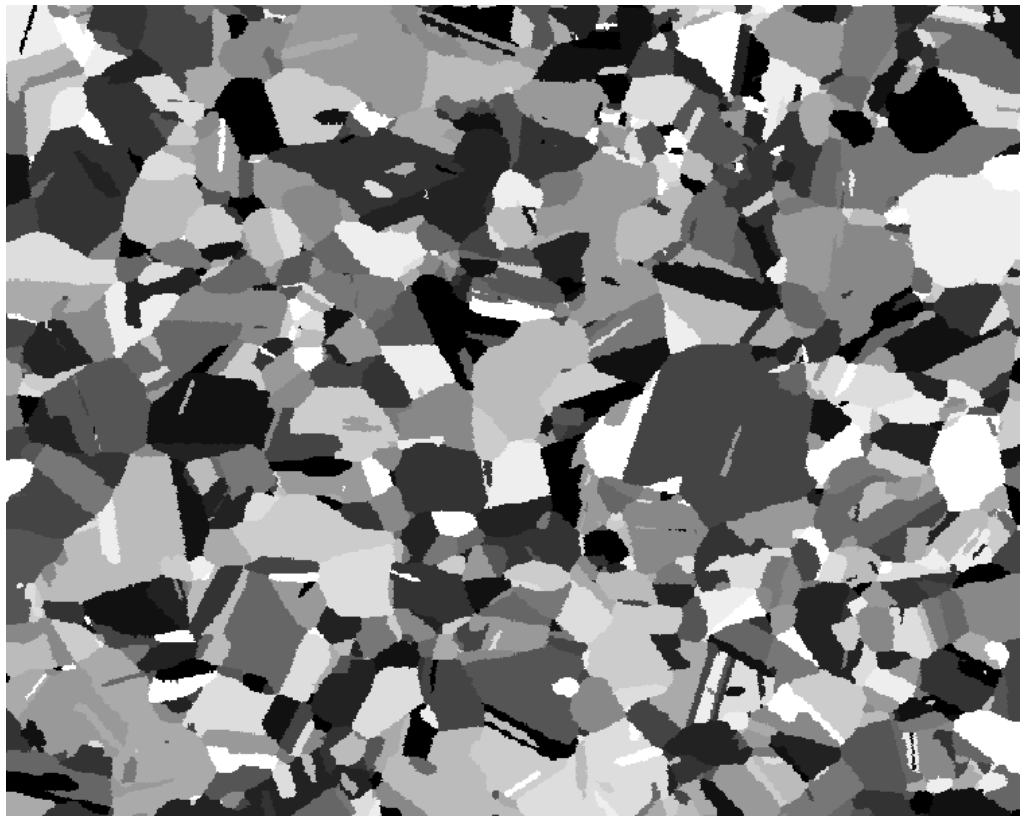
Grain evolution (Hillert's theory)

$$R_i \frac{dR_i}{dt} = M\gamma\beta\left(\frac{R_i}{R_{cr}} - 1\right)$$

Development of an algorithm for the immersion of experimental images

The big challenge:

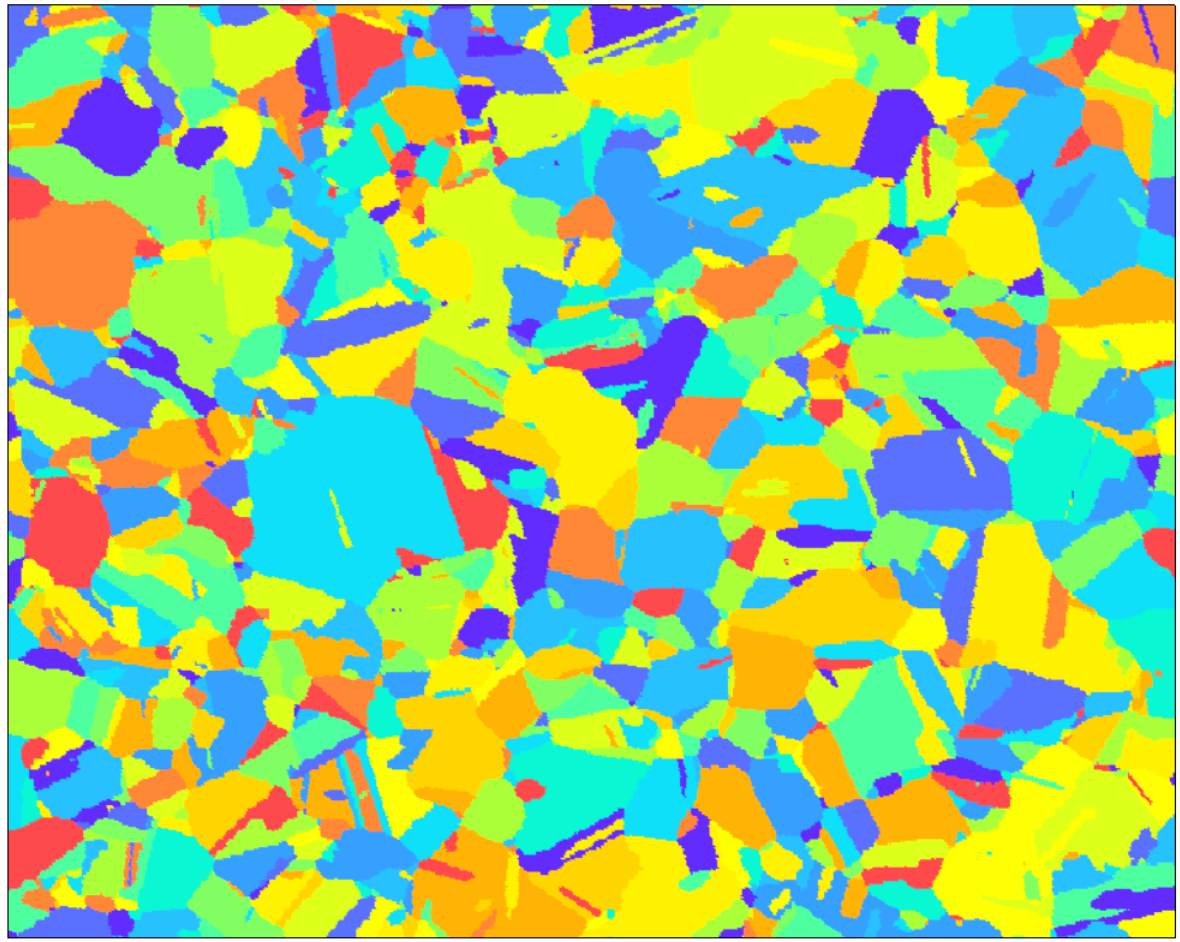
- From that...



Problem statement

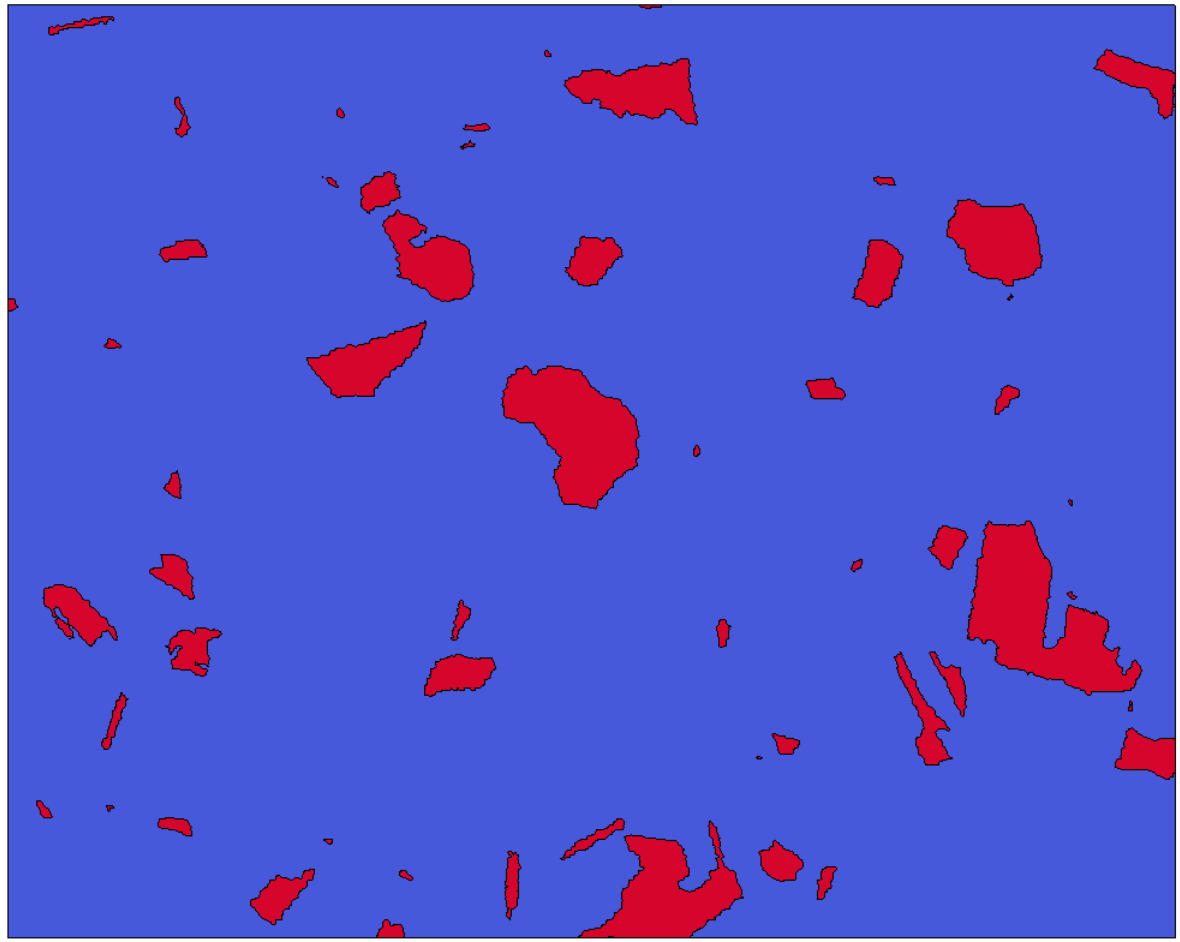
How to initialize the LS functions and distribute the grain in them?

Coloring of the experimental microstructure



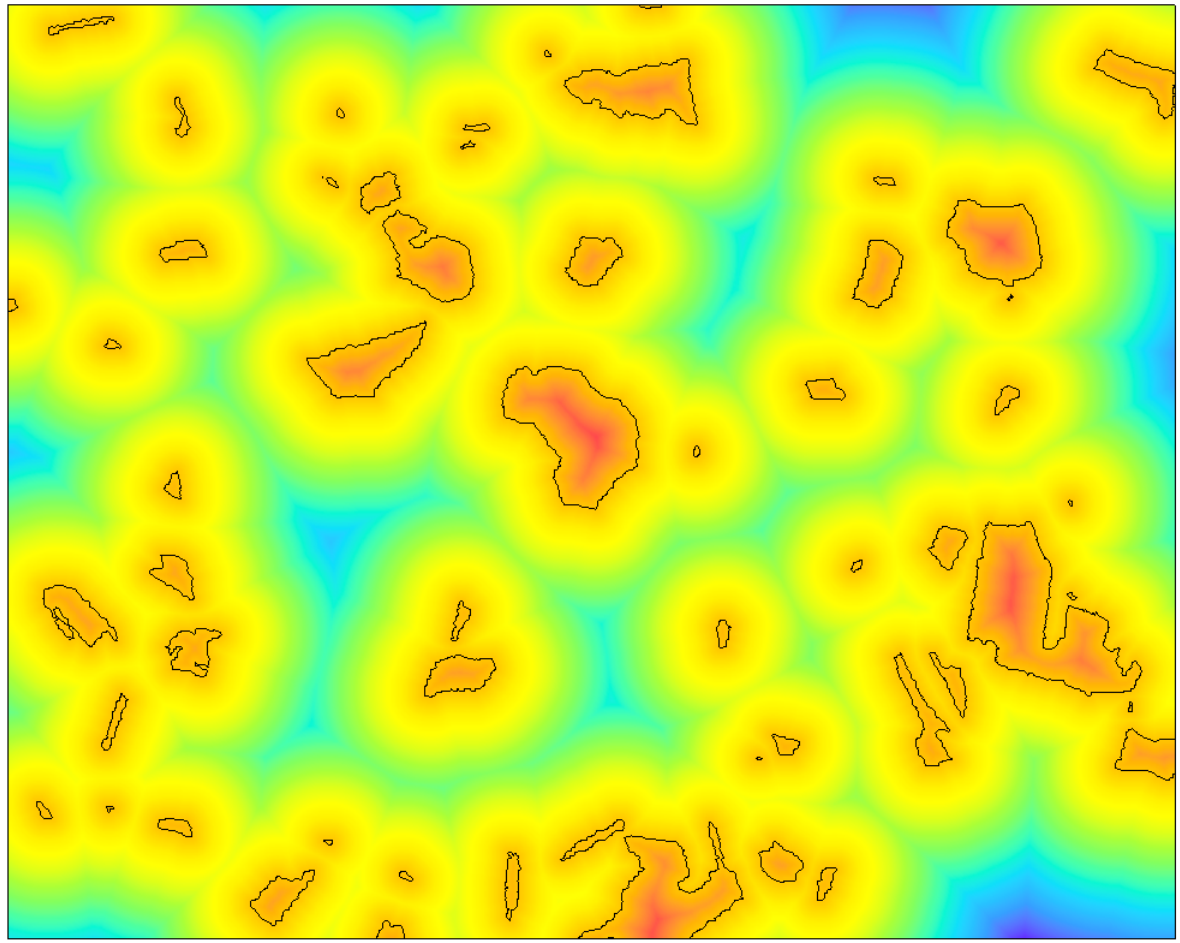
Coloring of the initial immersed microstructure obtained by scanning the pixels/voxels of the image and by applying the coloring algorithm developed in (Hitti, PhD 2011). The color of each grain refers to the index of the GLS function that represent this grain

Binary representation of each LS functions



Initialization of each LS function as a binary field, based on the previously established coloring

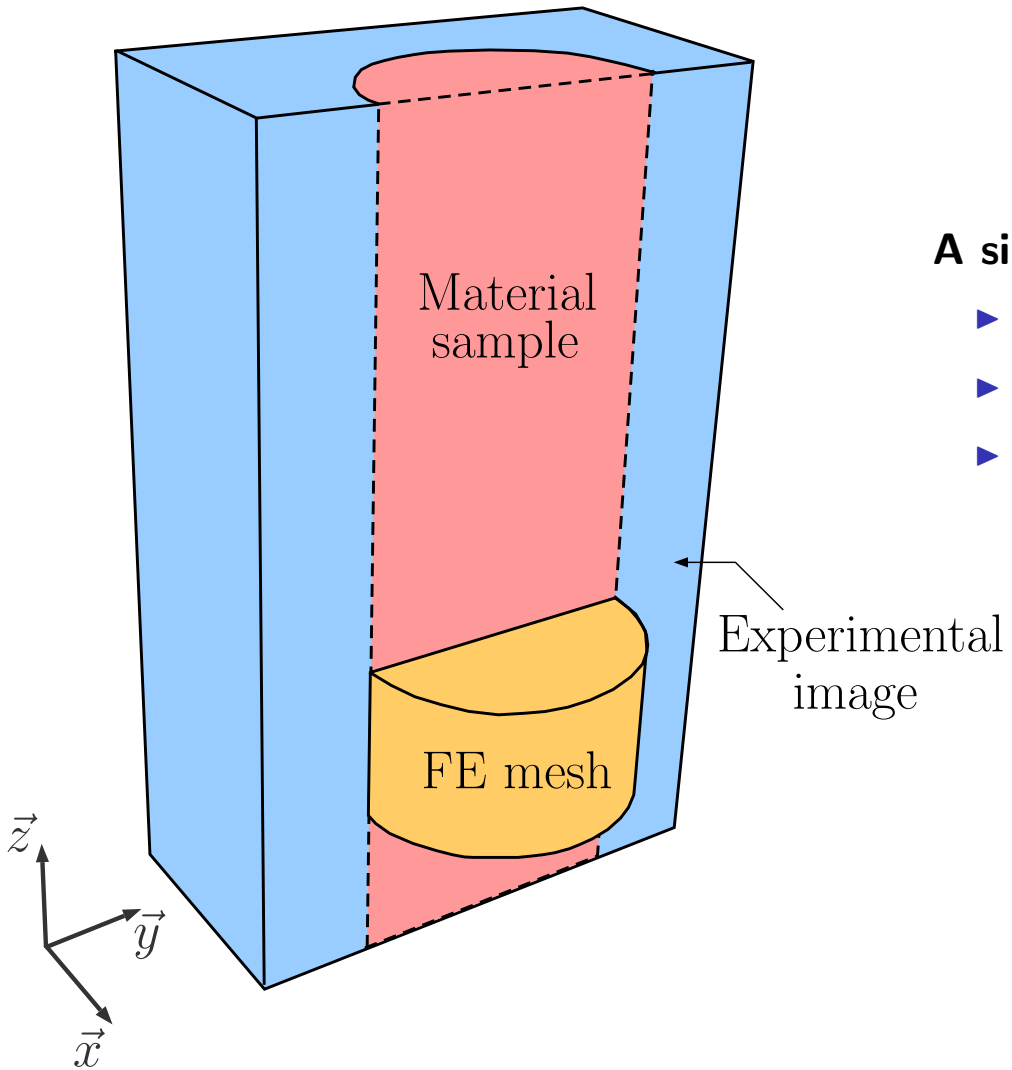
Binary representation of each LS functions



Creation of the LS function based on the binary field by using the reinitialization algorithm developed in (Shakoor et al. 2015)

M. Shakoor, B. Scholtes, P.-O. Bouchard, M. Bernacki "An efficient and parallel level set reinitialization method - Application to micromechanics and microstructural evolutions", *Applied Mathematical Modelling* (2015)

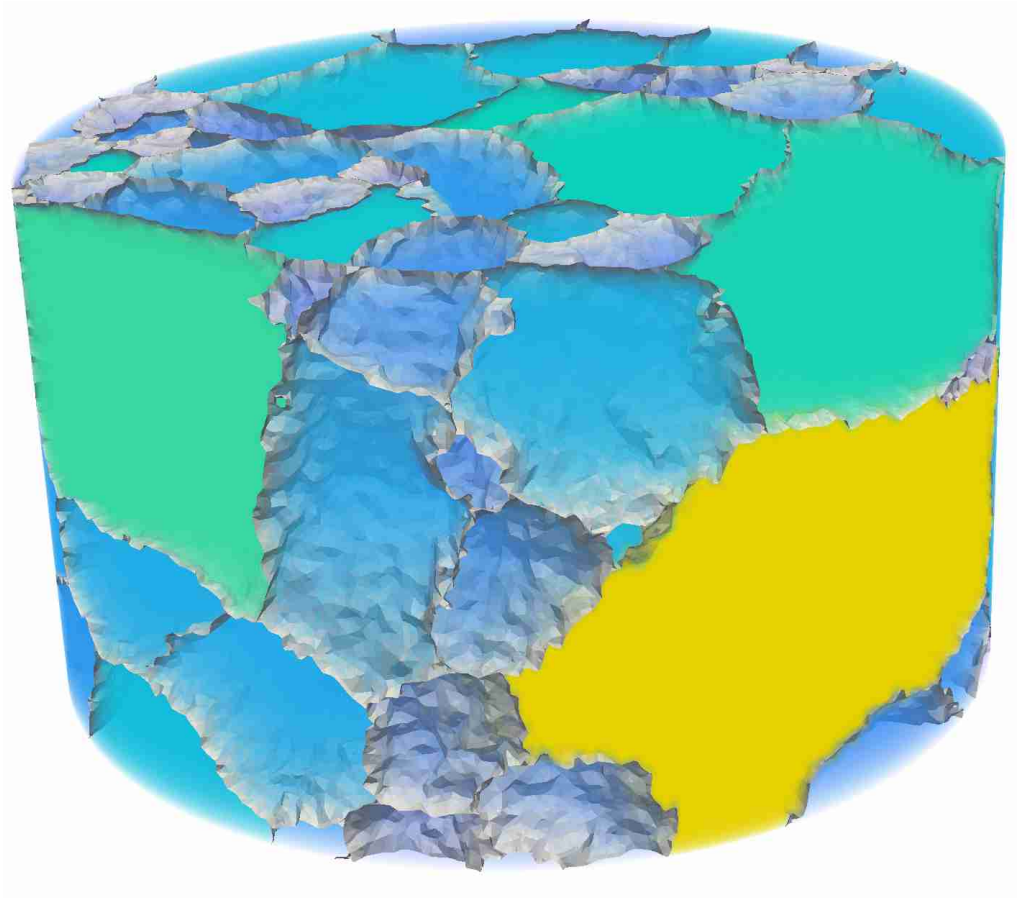
Immersion from a 3D experimental image



A simple grain growth case

- $321 \times 321 \times 531$ voxels data box
- 1300 grains in the cylindrical sample
- Material: aluminum

Immersion from a 3D experimental image

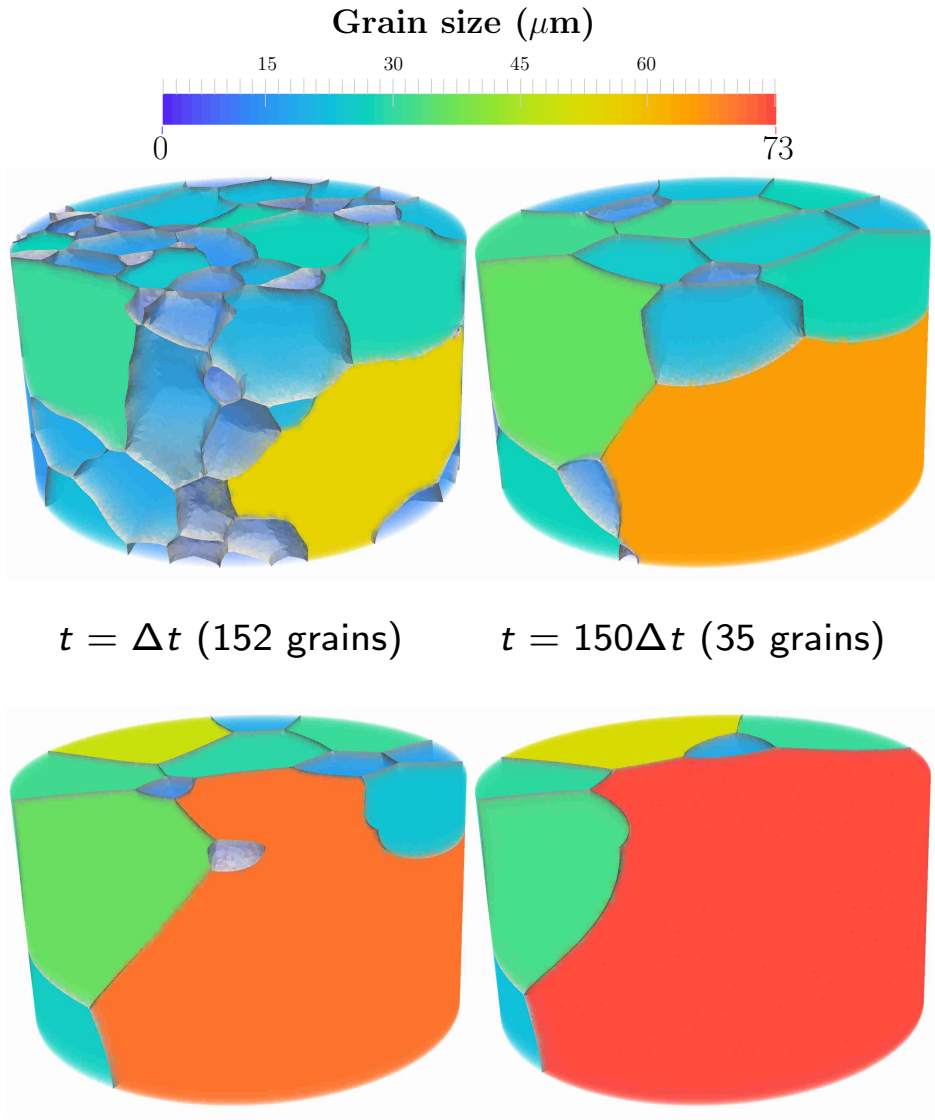


Immersion of a portion of the aluminum sample within a cylindrical FE mesh

Simulation from a 3D experimental image

Heat treatment simulation

- 17min of heat treatment with $M\gamma = 1\mu\text{m}^2/\text{s}$ (arbitrary value)
- Initial polycrystal composed of 150 grains
- Material : aluminum

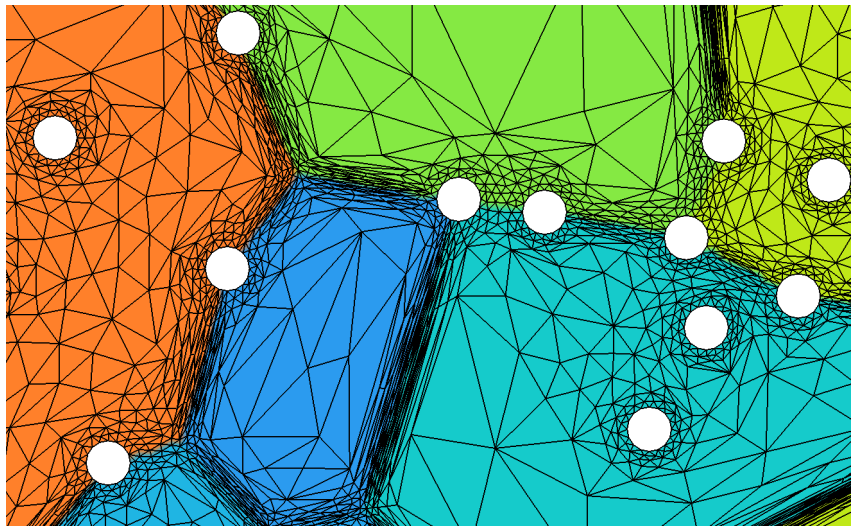


$t = \Delta t$ (152 grains) $t = 150\Delta t$ (35 grains)

$t = 3000\Delta t$ (22 grains) $t = 450\Delta t$ (10 grains)

Current methodology for the modeling of second phase particles

- Before the simulation, create a FE mesh which contains holes representing the SPP
- Apply suitable boundary conditions on the corresponding SPP faces (null boundary condition for incoherent particles $\rightarrow$ normal interaction angle)
- The grain boundaries will then be naturally slowed down by the modification of their local curvature

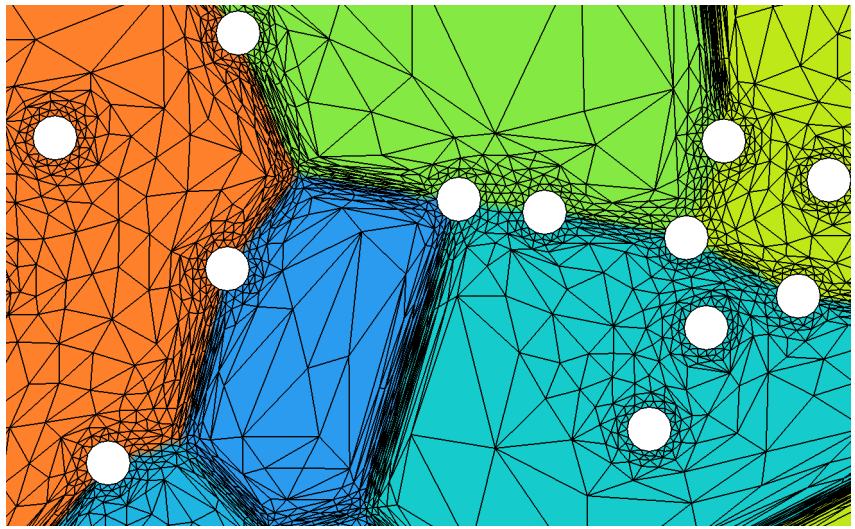


Agnoli et al. "Development of a level set methodology to simulate grain growth in the presence of real secondary phase particles and stored energy" *Comp. Mat. Sci.* (2013)

B. Scholtes, D. Ilin, A. Settefrati, N. Bozzolo, A. Agnoli, M. Bernacki "Full field modeling of the Zener pinning phenomenon in a level set framework - discussion of classical limiting mean grain size equation" *Submitted in Superalloys 2016: 13th International Symposium on Superalloys* (2016)

Current methodology: advantages and limitations

- With the exception of the mesh, no modification compared to a simulation without particles
- 1 mesh = particle cloud $\rightarrow$ require the creation of specific mesh for each particle distribution
- Very complicated (even impossible with our current numerical tools) to handle evolving particles



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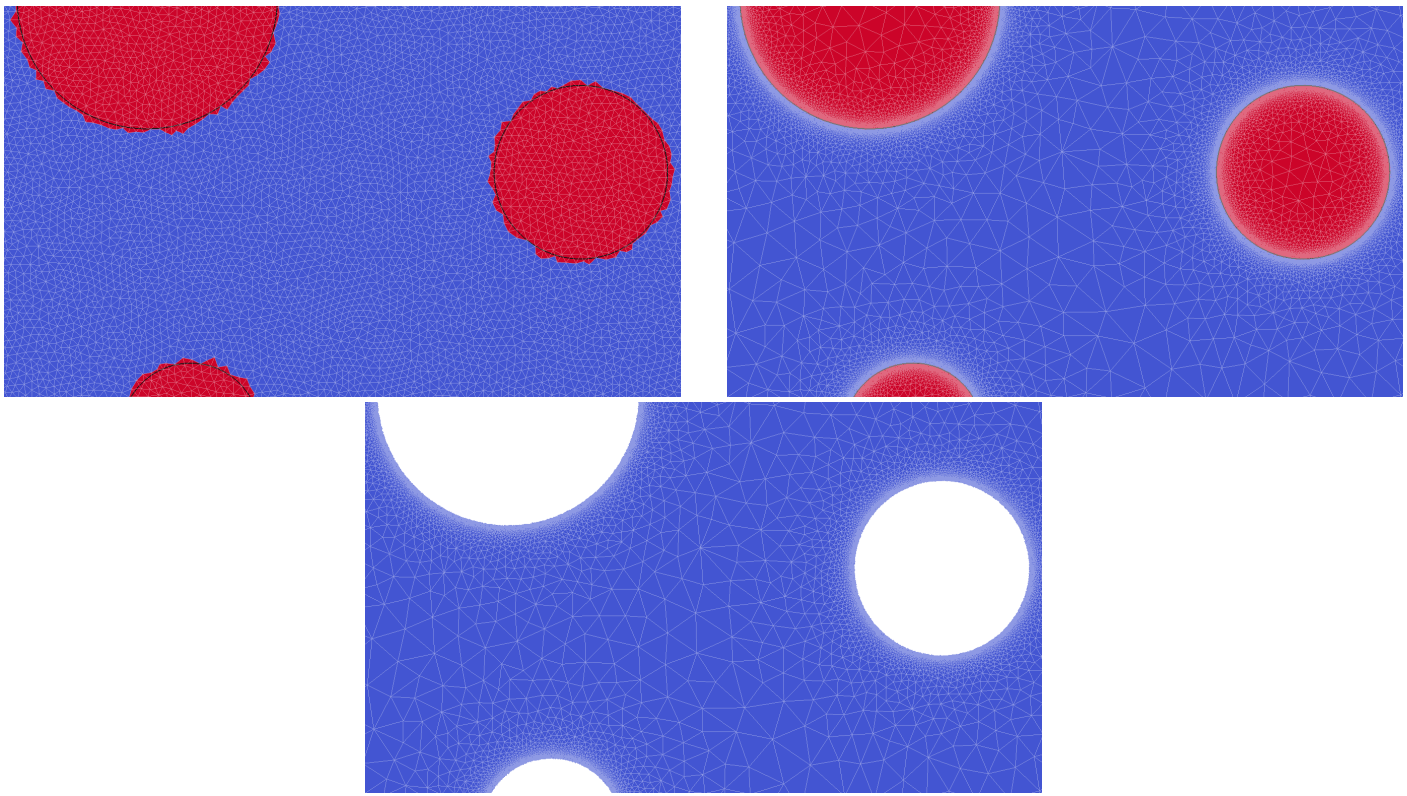
Existing approach for the generation of the Zener pinning FE meshes

- Create a field that represent the particles (binary field or distance field)
- If needed, refine the mesh at the interface of the particles
- *Kill* the elements and nodes located inside the particles



Limitations of this approach

- Relies on mesh adaptation $\rightarrow$ high computation cost
- Accuracy of the precipitate description depends on the number of elements used to perform the mesh adaptation and/or the prescribed mesh sizes

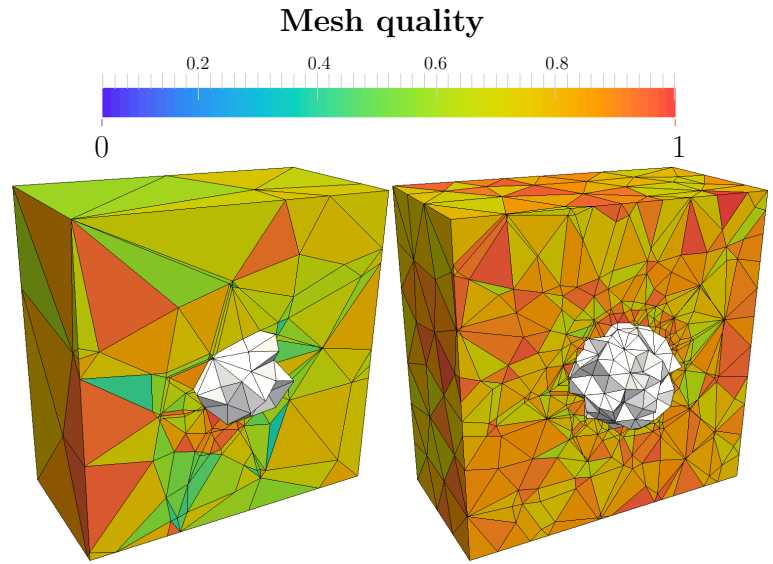
Let us take a simple illustrating example

FE mesh generation for a single precipitate

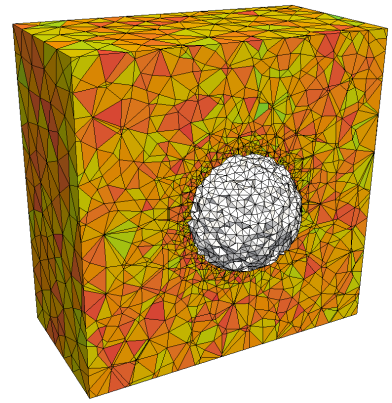
- $r_p = 0.35\mu$m, representative of Inconel 718 (Agnoli et al. 2014)
- Domain dimension $2 \times 2 \times 2\mu\text{m}^3$, which gives $f_v = 2\%$, representative of Inconel 718 (Agnoli et al. 2014)
- Different mesh sizes are testes near the precipitate ($r_p/2$, $r_p/5$, $r_p/10$)
- The generated FE meshes and the CPU times are compared, using 1 CPU

	Coarse	Medium	Fine
Number of elements	718	3324	32354
CPU time for one particle	9.2s	12.8s	52.2s
Estimate CPU time for 10000 particles	1 day 2h	1 day 12h	6 days 1h

10000 particles is for a 500 grains Inconel polycrystal with initial grain size $\langle R_0 \rangle = 3.5\mu$m



Coarse (718 elements) Medium (3324 elements)



Fine (32354 elements)

Development of a new approach (GBMG) for generating Zener pinning FE meshes

- Generate a dispersoid of spheres (respectively disks in 2D) in the simulation domain, that satisfies the prescribed volume fraction fraction and the prescribed size distribution of the SPPs. This is done by using the algorithm developed by Hitti (Hitti 2011, Hitti et al. 2016) which generates the centers and radii of the precipitates and allows to each easily high density but also to handle particle clustering,

- Create a geometric description of the particle cloud (points, lines, splines, surfaces, volumes) that can be understood by the mesh generator

- Mesh the geometric entities in the order of dimensionality according to a frontal algorithm (GMSH)

- Post-treat the generated mesh file in order to make it compatible with our C++ library.

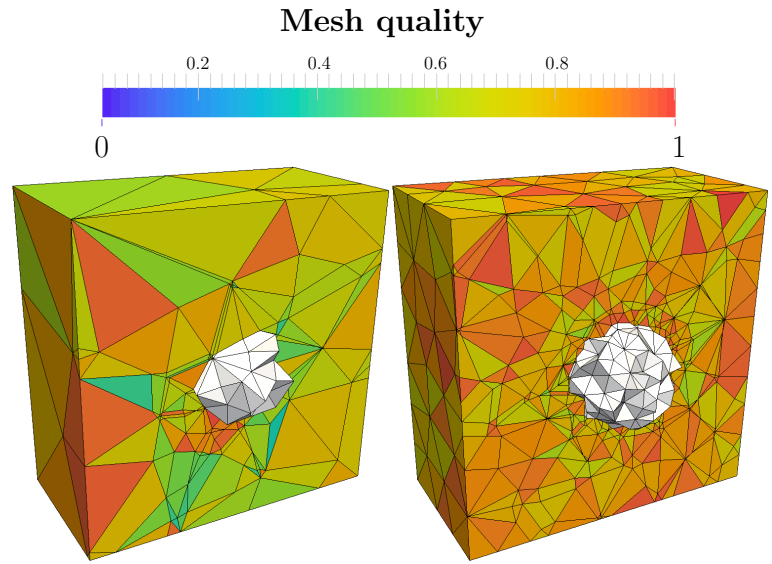
Let us go back to the single precipitate example

FE mesh generation for a single precipitate

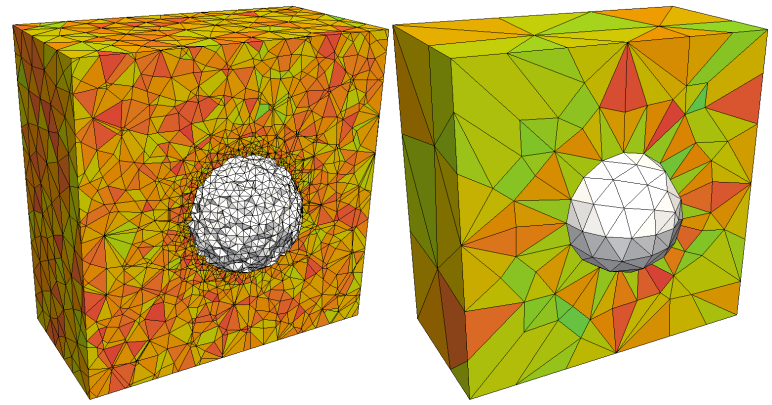
- $r_p = 0.35\mu$m, representative of Inconel 718 (Agnoli et al. 2014)
- Domain dimension $2 \times 2 \times 2\mu\text{m}^3$, which gives $f_v = 2\%$, representative of Inconel 718 (Agnoli et al. 2014)
- Different mesh sizes are testes near the precipitate ($r_p/2$, $r_p/5$, $r_p/10$)
- The generated FE meshes and the CPU times are compared, using 1 CPU

	Coarse	Medium	Fine
Number of elements	718	3324	32354
CPU time for one particle	9.2s	12.8s	52.2s
Estimate CPU time for 10000 particles	1 day 2h	1 day 12h	6 days 1h

With GBMG: only 117ms $\rightarrow$ 80 times faster than the "Coarse" case with far better quality



Coarse (718 elements) Medium (3324 elements)

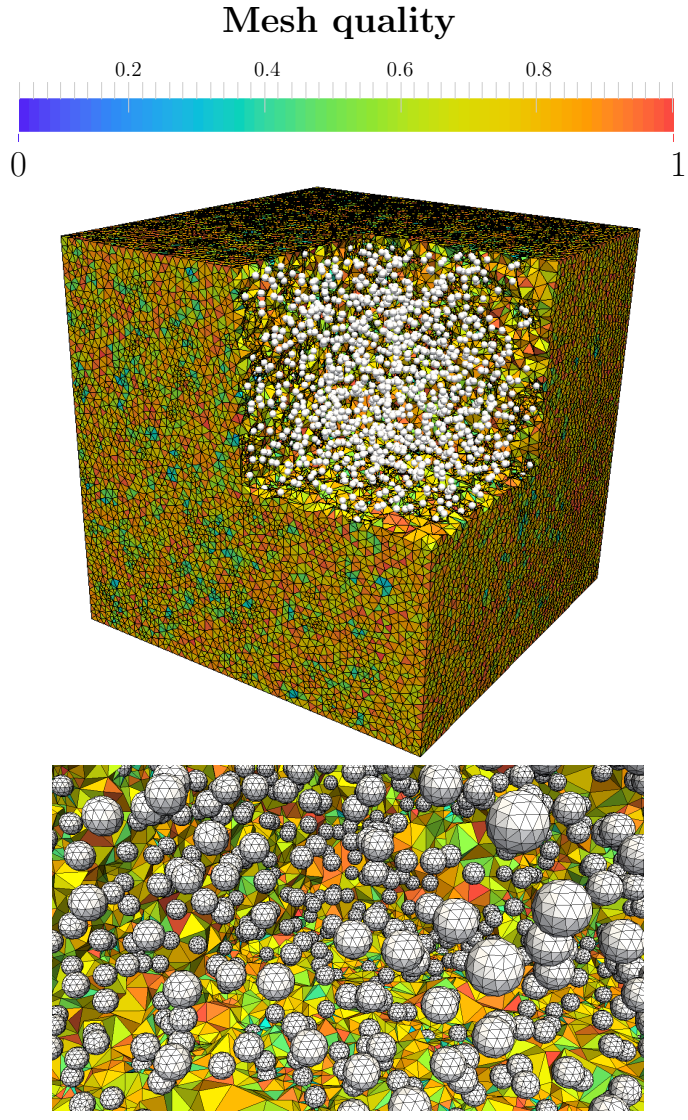


Fine (32354 elements) GBMG (755 elements)

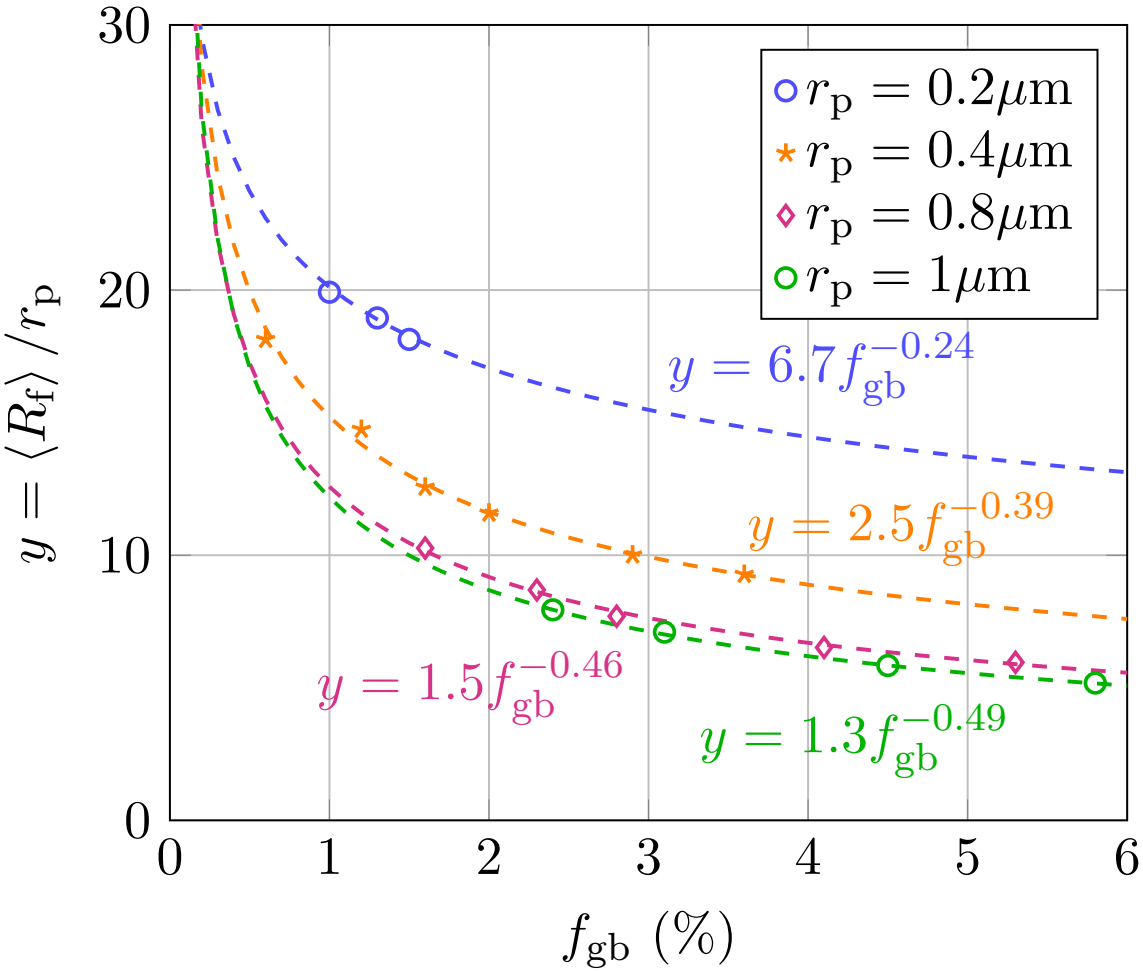
Generation of a massive 3D mesh

FE mesh generation for big cloud precipitates

- $r_p = 0.35\mu$m, representative of Inconel 718 (Agnoli et al. 2014)
- 10000 particles
- Domain dimension $44 \times 44 \times 44\mu\text{m}^3$, which gives $f_v = 2\%$, representative of Inconel 718 (Agnoli et al. 2014)
- Final mesh contains 7 million elements
- 40min needed to generate this mesh, using 1 CPU

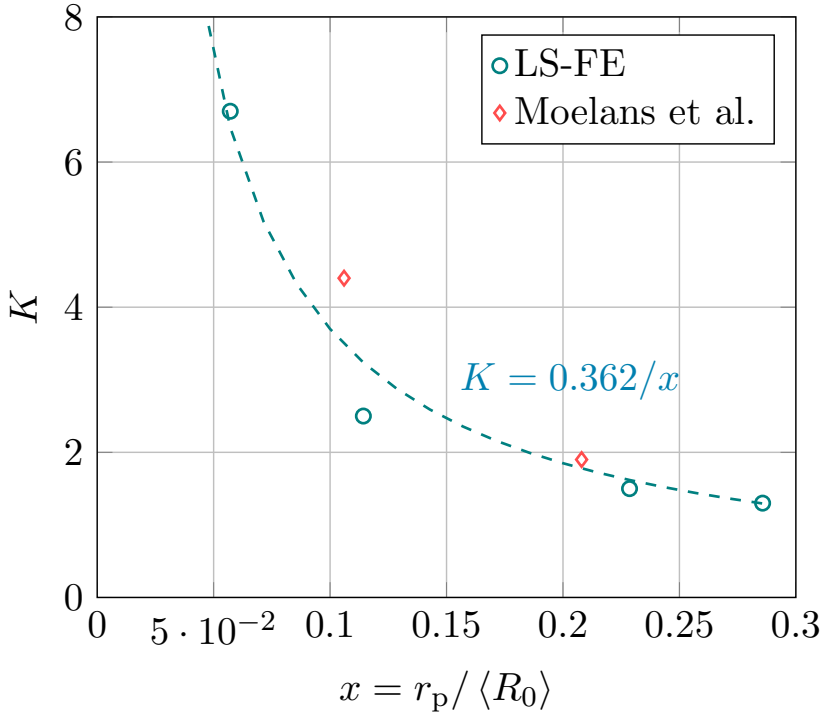


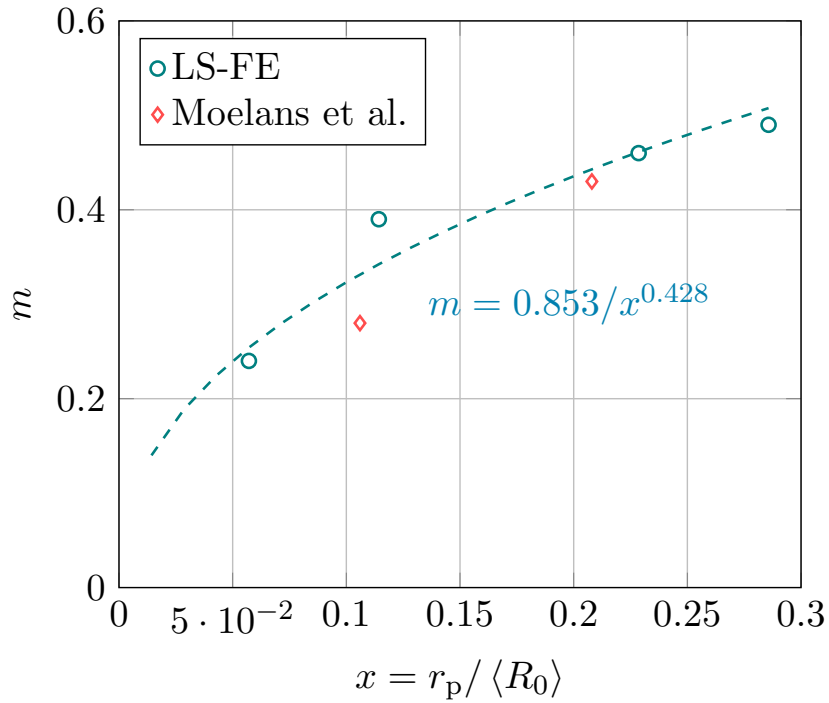
Results of full field simulations



Results of 2D pinning simulations for Inconel 718 with different particle volume fractions and radiuses. Each point is the result of a full field simulation.

Results of full field simulations





Evolution of the fitting parameters (K;m) of the limiting mean grain size obtained with the full field simulation results.

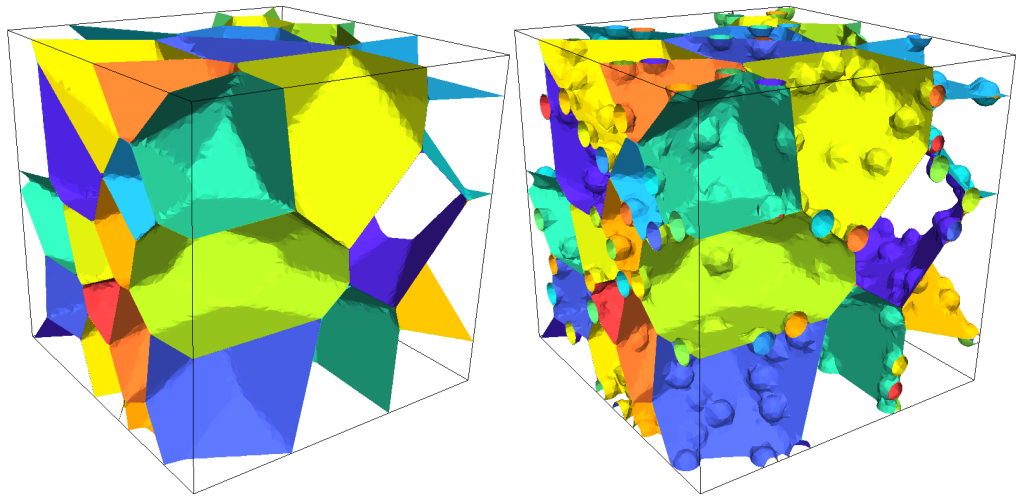
Moelans et al. "Phase field simulations of grain growth in two-dimensional systems containing finely dispersed second-phase particles" *Acta Mat.* (2006)

B. Scholtes, D. Ilin, A. Settefrati, N. Bozzolo, A. Agnoli, M. Bernacki "Full field modeling of the Zener pinning phenomenon in a level set framework - discussion of classical limiting mean grain size equation" *Submitted in Superalloys 2016: 13th International Symposium on Superalloys* (2016)

Anisotropic mesh adaptation

Mesh adaptation in 3D

Non linearity of the simulation time



	Without coloring	C_1 criterion	C_2 criterion
$\langle N_p \rangle$	343	90	21
Solving of CDEs (see Eq. 5)	7h09min	1h56min	27min
Reinitialization	2h01min	1h02min	38min
Others	37min	8min	3min
Total simulation time	9h47min	3h06min	1h08min

$$\frac{t_s - t_s^{C_2}}{t_s^{C_2}} = 0.5 \frac{\langle N_p \rangle - \langle N_p \rangle^{C_2}}{\langle N_p \rangle^{C_2}}$$

Most significant publications

- *An efficient and parallel level set reinitialization method - application to micromechanics and microstructural evolutions*, M. Shakoor, B. Scholtes, P.-O. Bouchard, M. Bernacki, **Applied Mathematical Modeling** (2015)
- *New finite element developments for the full field modeling of microstructural evolutions using the level set method*, B. Scholtes, M. Shakoor, A. Settefrati, P.-O. Bouchard, N. Bozzolo, M. Bernacki, **Computational Materials Science** (2015)
- *3D level set modeling of static recrystallization considering stored energy fields*, B. Scholtes, R. Boulais-Sinou, A. Settefrati, D. Pino Munoz, I. Poitrault, A. Montouchet, N. Bozzolo, M. Bernacki, **Computational Materials Science** (2016)
- *Improvement of 3-D mean field models for capillarity driven grain growth based on full field simulations*, L. Maire, B. Scholtes, C. Moussa, N. Bozzolo, D. Pino Munoz, M. Bernacki, **Journal of Materials Science** (2016)
- *Full field modeling of the Zener pinning phenomenon in a level set framework - discussion of classical limiting mean grain size equation*, B. Scholtes, D. Ilin, A. Settefrati, N. Bozzolo, A. Agnoli, M. Bernacki, **Superalloys 2016: 13th International Symposium on Superalloys** (2016)
- Probably one more article concerning the numerical modeling of the HIP bounding process (publication of the polycrystal immersion procedure and of the new techniques for generating Zener pinning FE meshes)

International conferences

- *Advances in level set modeling of recrystallization at the mesoscopic scale development of the digi- software*, B. Scholtes, A. Settefrati, M. Bernacki, in **CAE conference**, Verona, Italy (2014)
- *Advances in level-set modelling of recrystallization at the microscopic scale development of the digi- software*, B. Scholtes, M. Shakoor, N. Bozzolo, P.-O. Bouchard, A. Settefrati, M. Bernacki, in **ESAFORM 2015**, Graz, Austria (2015)
- *Recent advances in the full field modeling of recrystallization and grain growth using the level set approach*, B. Scholtes, A. Settefrati, M. Bernacki, in **EUROMAT 2015**, Warsaw, Poland (2015)
- *3D Full field modeling, in a level set framework, of grain growth and zener pinning phenomenon*, M. Bernacki and B. Scholtes, in **EUROMAT 2015**, Warsaw, Poland (2015) - Invited conference, keynote
- *New finite element developments for the full field modeling of microstructural evolutions using the level set method*, B. Scholtes, A. Settefrati, M. Bernacki, **WCCM XII: The 12th world Congress on Computational Mechanics**, Seoul, Korea (2016)