Centre de Mise en Forme des Matériaux

High Performance Computing to Improve Understanding of Materials Science

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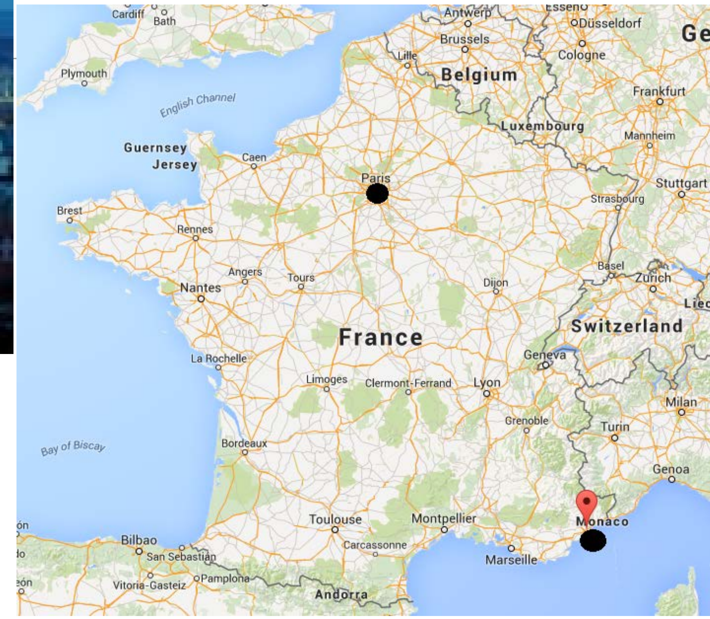
Marc Bernacki, Pierre-Olivier Bouchard, Elie Hachem

TERATEC 2016



Cemef

« Materials Forming Center »

160	People
60	Permanent staff (1/2 researchers)
70	PhD students

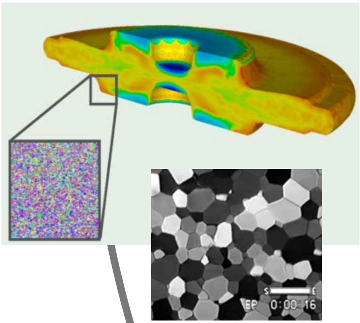
Outline

- Unified framework
  - Geometric representation by a levelset
  - Mesh adaptation
  - Stabilized finite element resolution

- Grain growth simulation
- Damage-Fracture & Void Closure
- Application to conjugate heat transfer
- Miscellaneous

- Concluding remarks

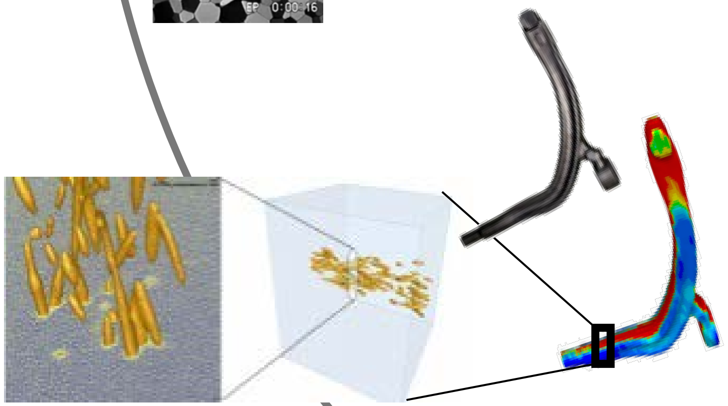
Driven by industrial needs



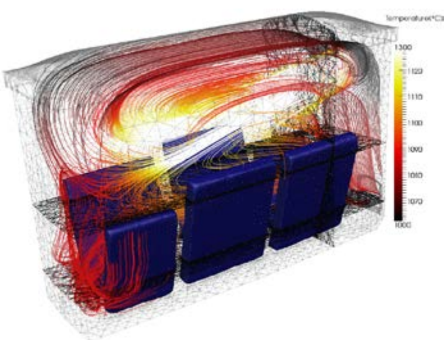
meso scale

Material Forming

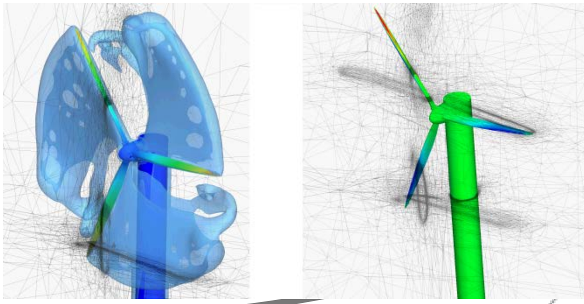
- Need to understand new physical phenomena
- Building a bridge between scales
- Thermo mechanical analyses
- Process optimization
- Flexibility to deal with different geometries



Different solutions:
- Partitioned Approaches [Wall WA, 1999]
- Fictitious domain [Glowinski R, 1999]
- Immersed Boundary (IB) [Peskin CS, 2002]
- Monolithic approach [Fedkiw C, 2010]
- Embedded methods [Farhat C, 2011]



large scale



Common numerical tools:

- Level set representation
- Mesh adaptation
- Stabilized finite element methods

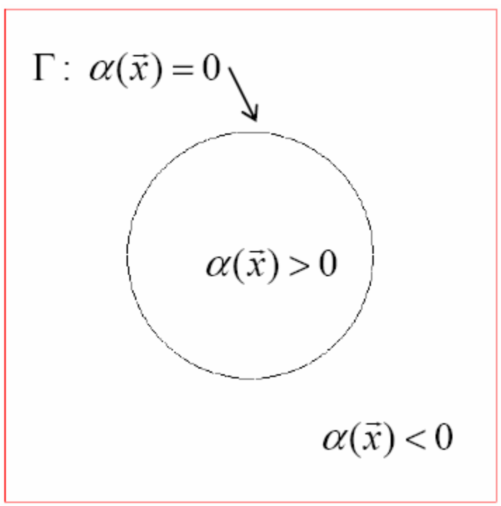
Immersed Volume Method: the basic idea

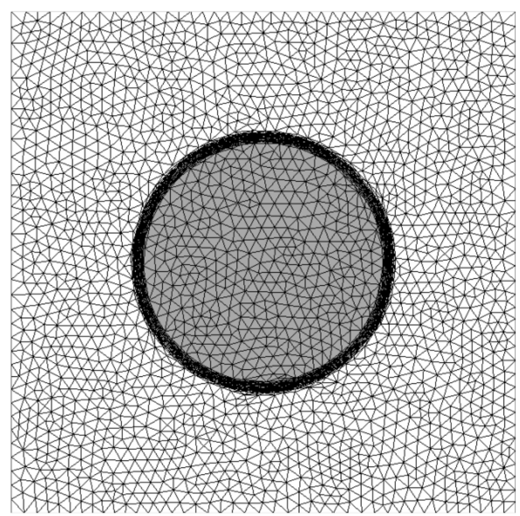
- ✓ We compute the distance function
- ✓ We sign it to obtain the LevelSet function
- ✓ We apply anisotropic mesh adaptation using the gradients of the levelset function
- ✓ We regularize it over a certain thickness ε and use it to mix the physical properties

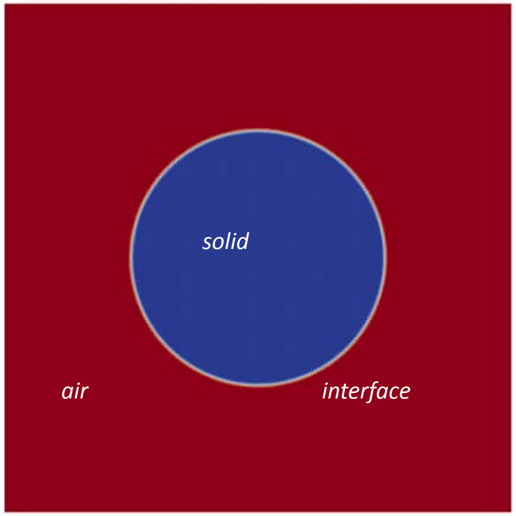
$$\alpha(\mathbf{x}) = \pm d(\mathbf{x}, \Gamma_{\mathrm{im}}), \mathbf{x} \in \Omega,$$
$$\Gamma_{\mathrm{im}} = \{\mathbf{x}, \alpha(\mathbf{x}) = 0\}.$$

$$H_\varepsilon(\alpha) = \begin{cases} 1 & \text{if } \alpha > \varepsilon \\ \frac{1}{2}\left(1 + \frac{\alpha}{\varepsilon} + \frac{1}{\pi}\sin\left(\frac{\pi\alpha}{\varepsilon}\right)\right) & \text{if } |\alpha| \leq \varepsilon \\ 0 & \text{if } \alpha < -\varepsilon \end{cases}$$

$$\rho = H(\alpha)\rho_s + (1 - H(\alpha))\rho_f$$
$$\eta = H(\alpha)\eta_s + (1 - H(\alpha))\eta_f$$



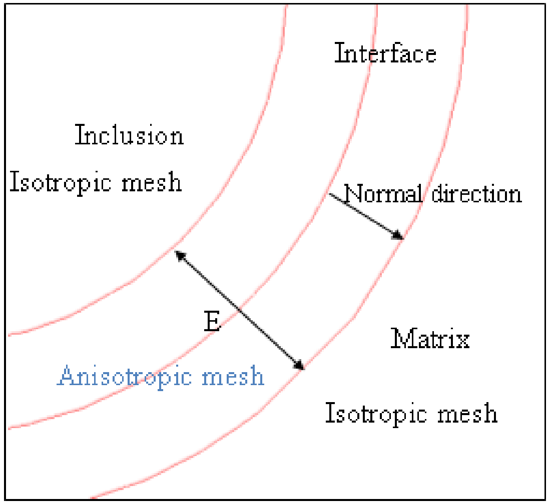




E. Hachem, E. Massoni, T. Coupez, ESAIM, ***2011***
E. Hachem, H. Digonnet, E. Massoni, T. Coupez, International Journal of Numerical Methods for Heat & Fluid Flow, ***2012***
E. Hachem , G. Jannoun, J. Veysset, M. Henri, R. Pierrot, I. Poitrault, E. Massoni, Simulation Modelling Practice and Theory, ***2013***

Anisotropic mesh adaptation

- A priori adaptation
  - Interfaces description
  - Metric based on the zero value of level-set functions: M_d



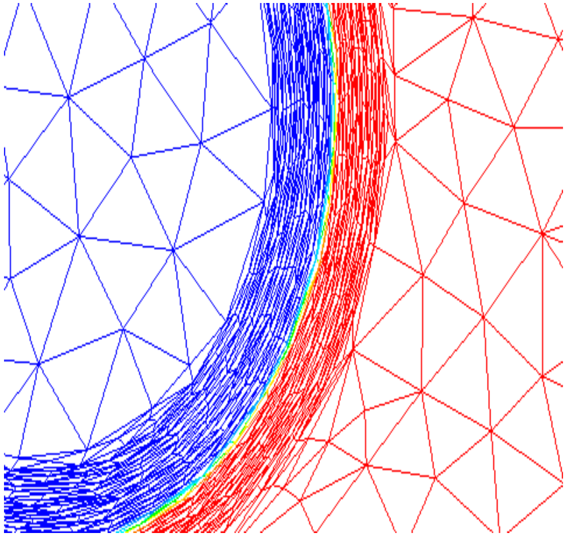
- A posteriori adaptation
  - Accuracy of the mechanical computation
  - Metric based on an a posteriori error estimator: M_m

- Combining both metrics

$$if \max_{i\in\{v,i,m\}}|\alpha_i(x)| < D_{\min} : M = M_d$$

$$if\ D_{\min} \le \max_{i\in\{v,i,m\}}|\alpha_i(x)| \le D_{\max} : M = \frac{M_d - M_m}{D_{\min} - D_{\max}}\left(\max_{i\in\{v,i,m\}}|\alpha_i(x)| - D_{\min}\right) + M_d$$

$$if\ D_{\max} < \max_{i\in\{v,i,m\}}|\alpha_i(x)| : M = M_m$$



[T. Coupez & E. Hachem, CMAME 2013]
[M. Bernacki et. al, MSMSE, 2009]

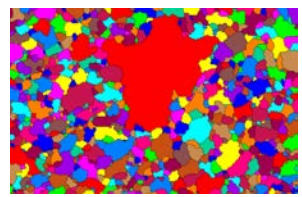
LevelSet convection

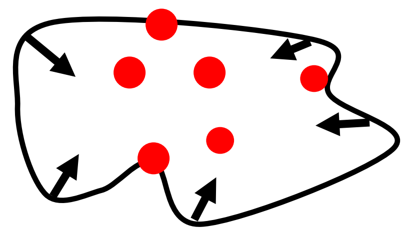
$$\frac{\partial \alpha_i}{\partial t} + \vec{v}.\vec{\nabla}\alpha_i = 0$$

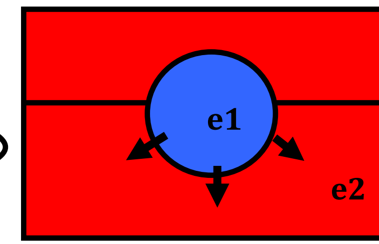
The velocity is obtained by solving Navier-Stokes using a Variational Multiscal Method

[T.J.R. Hugues et al.,1998]
[V. Gravemeier, W.A. Wall, 2004]
[R. Codina, 2002]
[E. Hachem et al, 2012]

The velocity is designed for grain boundary motion







$$\vec{v} = M(-\gamma\kappa + \Delta E)\vec{n}$$

- M: boundary mobility
- γ: boundary energy
- ΔE: stored energy

[Bernacki, 2011]
[Agnoli, 2014]
[Fabiano, 2014]

- Respect grain size distribution
- Respect second phase fraction and morphology
- Take into account capillarity effect
- Take into account the stored energy
- Deal with Zener Pinning

Grain boundaries motion rate equation

$$\vec{v} = M\Delta f\vec{n}$$

[Humphreys, 1995]

Grain boundary mobility

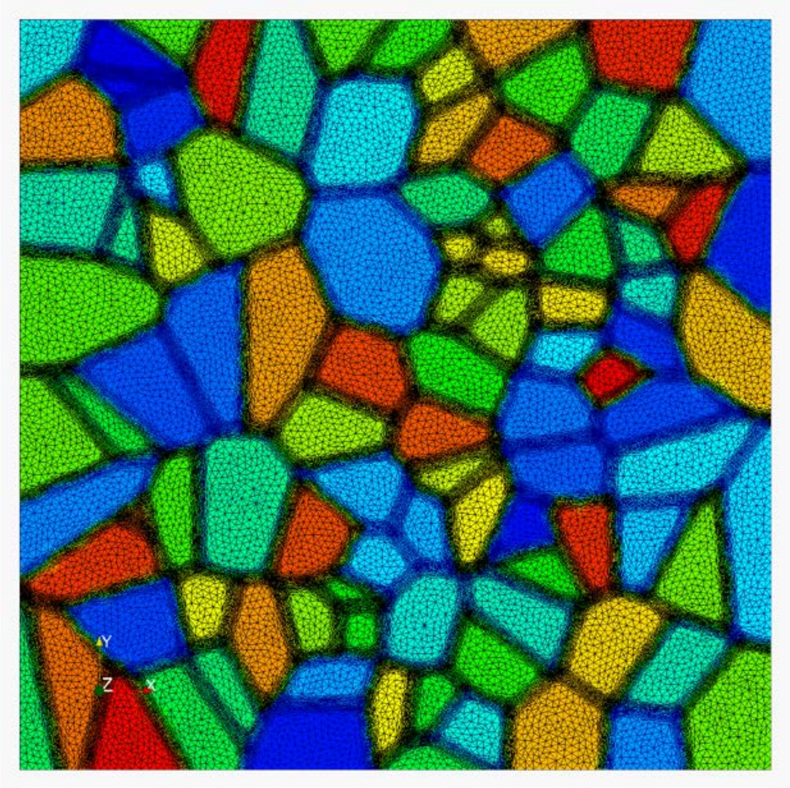
$$M = m_0(T)\exp\left(\frac{Q_b}{RT}\right)$$

Driving force per surface unit

$$\Delta f = \tau\Delta\rho - \gamma\kappa$$

Internal energy driving force

Mean grain boundary curvature driving force



τ → linear dislocation energy
$\Delta\rho$ → dislocation density
γ → grain boundary energy
κ → grain boundary curvature

Qb → activation energy
T → temperature
R → gas constant

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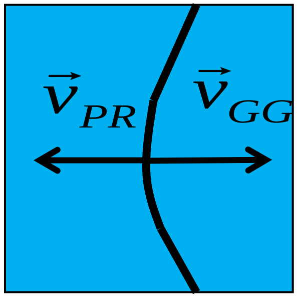
Used for Recrystallization formulation

Grain boundary motion simulation

$$\frac{\partial \alpha_i}{\partial t} + \left(\vec{v}_{GG_i} + \vec{v}_{PR_i}\right) . \vec{\nabla}\alpha_i = 0$$



$$\vec{v}_{GG_i} = -M_i \gamma_i \kappa_i \vec{n}_i$$

$$\vec{n}_i = \frac{\vec{\nabla}\alpha_i}{\left\|\vec{\nabla}\alpha_i\right\|}$$

$$\kappa_i = -\nabla . \left(\frac{\nabla \alpha_i}{\left\|\nabla \alpha_i\right\|}\right)$$

$$\left\|\vec{\nabla}\alpha_i\right\| = 1$$

$$\frac{\partial \alpha_i}{\partial t} + \vec{v}_{PR_i} . \nabla \alpha_i - M_i \gamma_i \Delta \alpha_i = 0$$

+

Solved using stabilized SUPG method [Hughes, 2001]

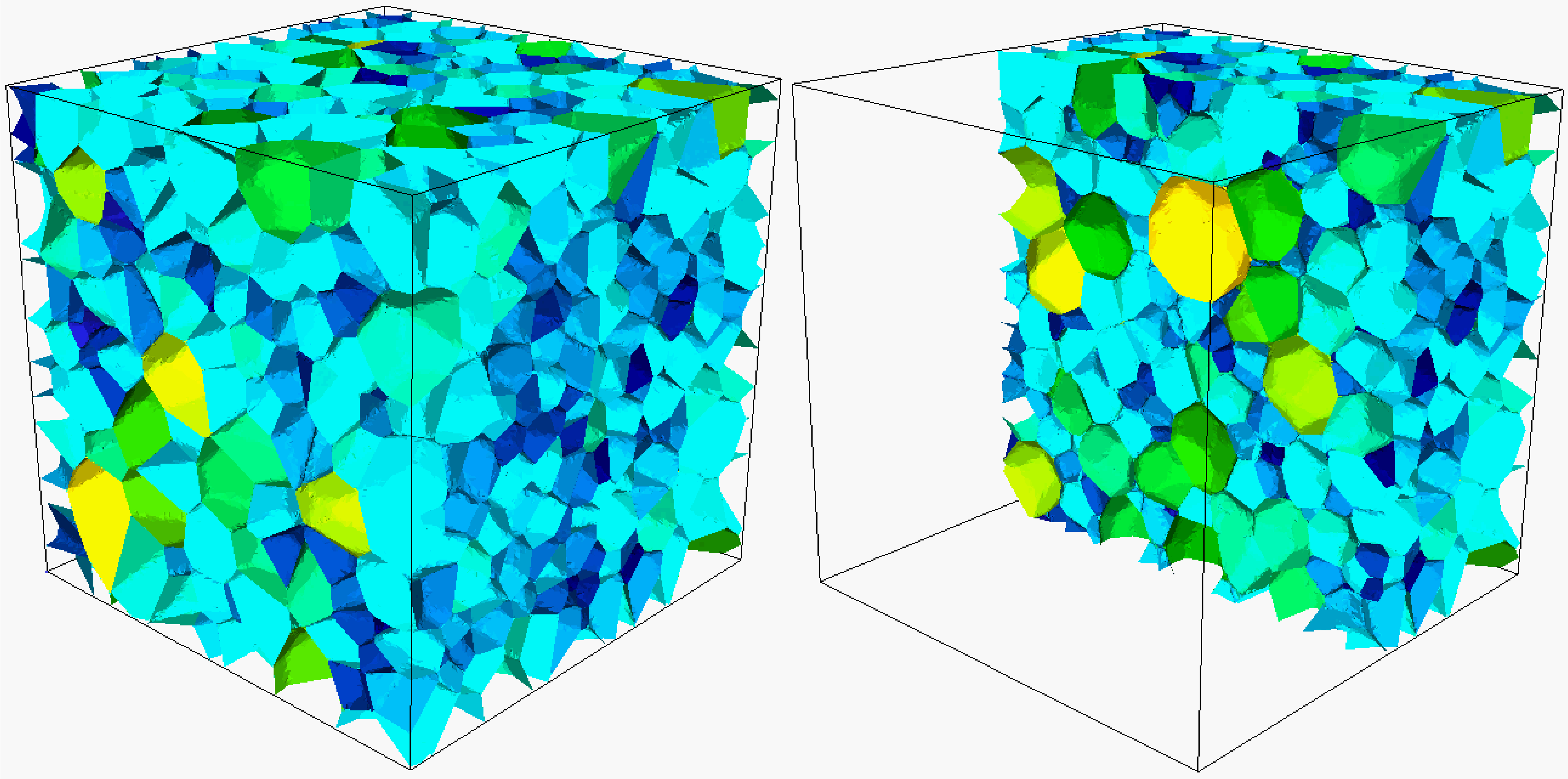
Treatment at multiple junctions

Geometric conservative re-initialization at each time step

Automatic anisotropic re-meshing operation

[Bernacki, 2011], [Fabiano, 2014]

3D Grain Grow Simulation



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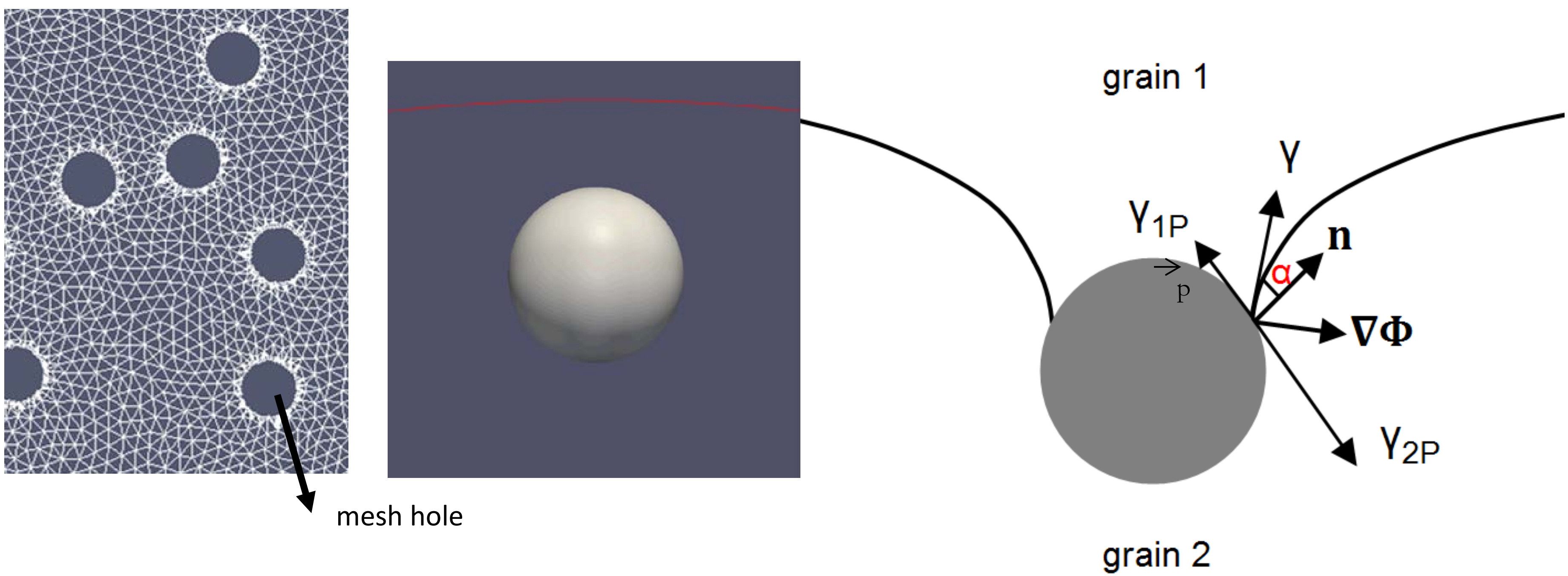
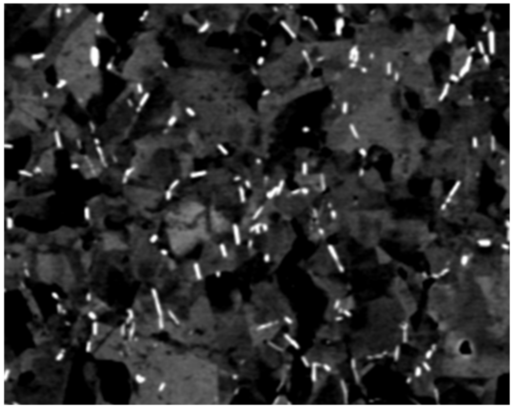
Zener Pinning

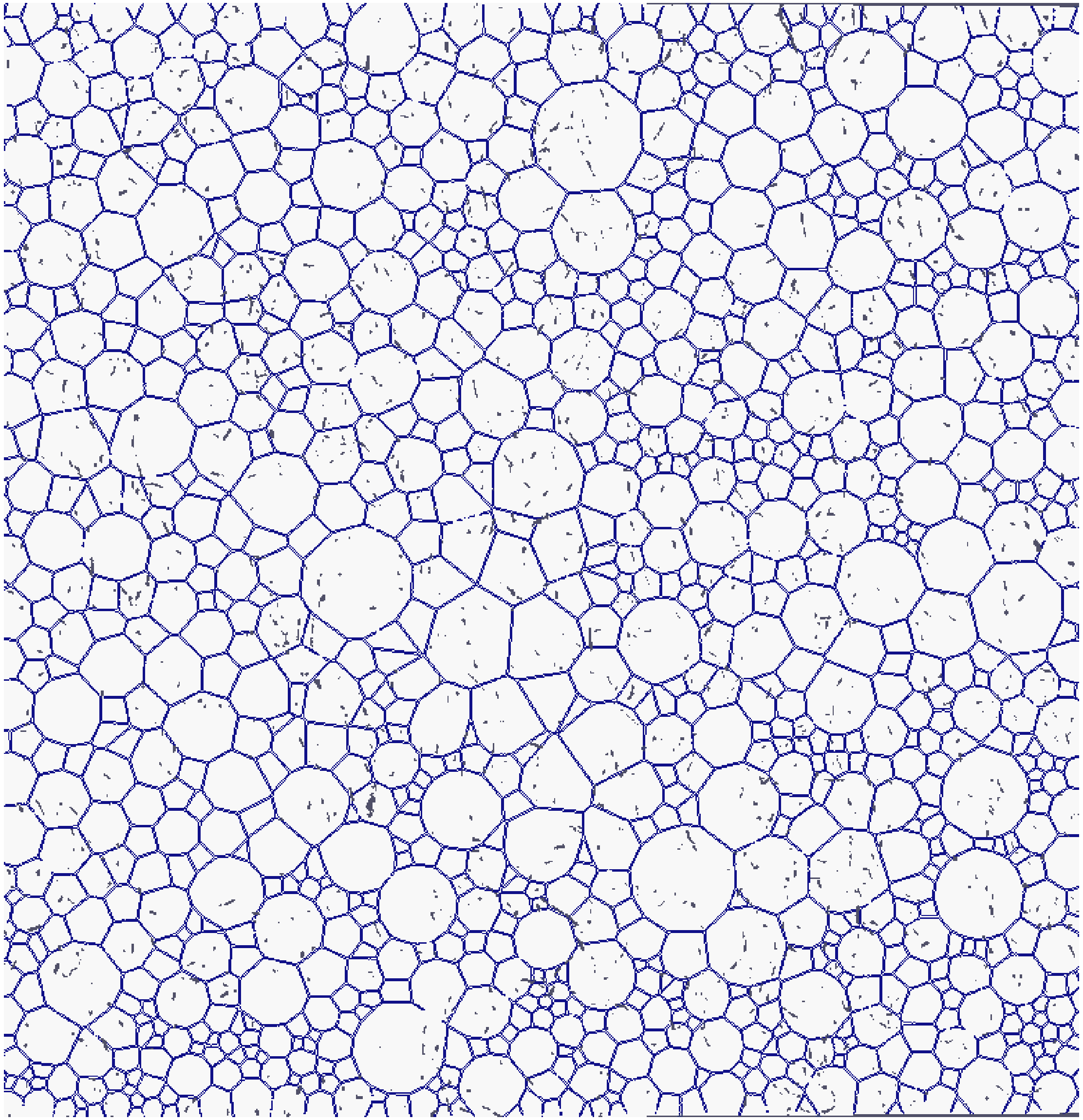
In a LevelSet context, the presence of particles is directly taken into account via the effect on boundary curvature
[Agnoli, 2013], [Agnoli, 2014]

$$\nabla\phi \cdot \vec{n}_{\mathrm{p}} = \sin(\alpha) = (\gamma_{2\mathrm{P}} - \gamma_{1\mathrm{P}})/\gamma$$

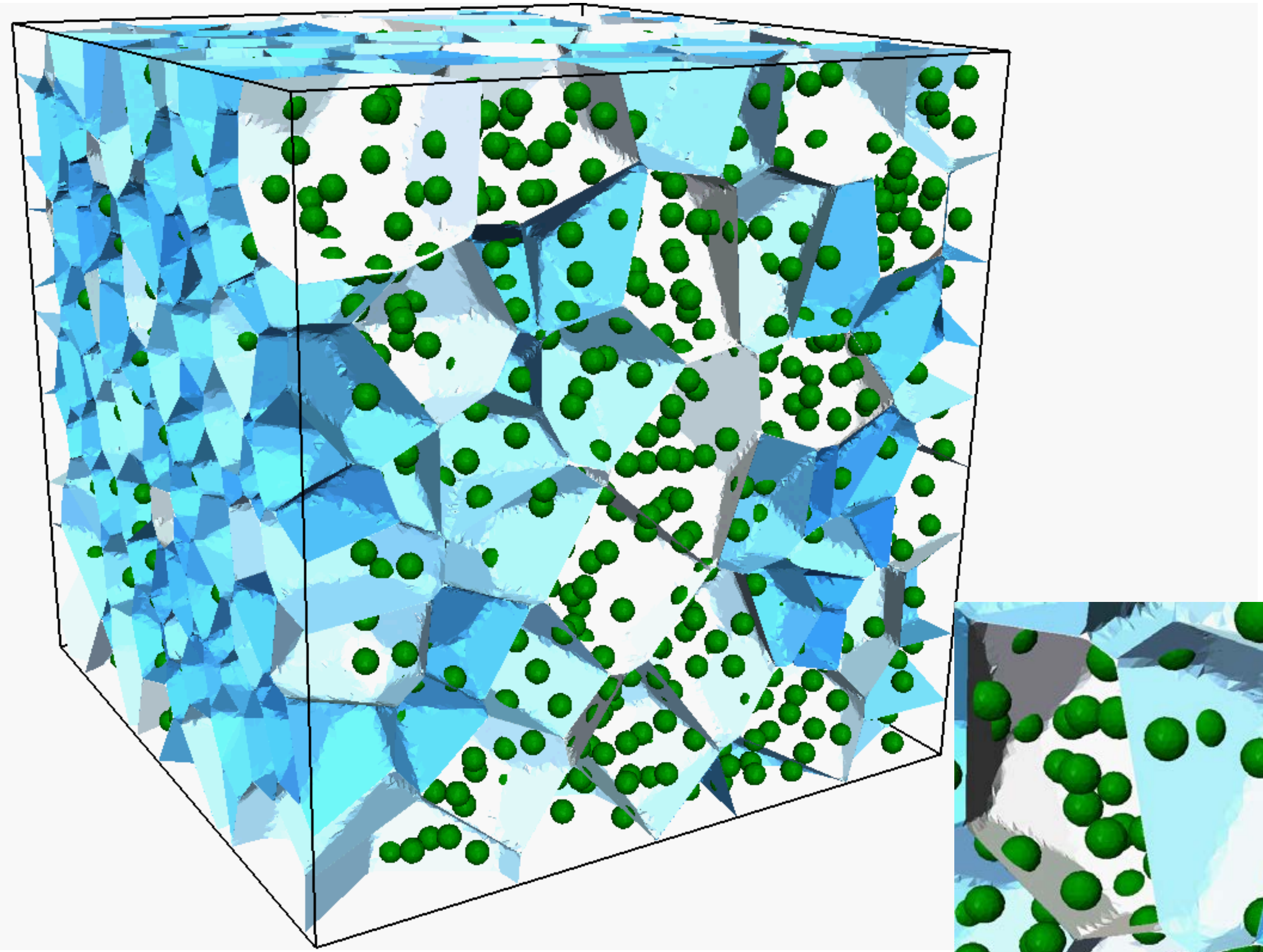


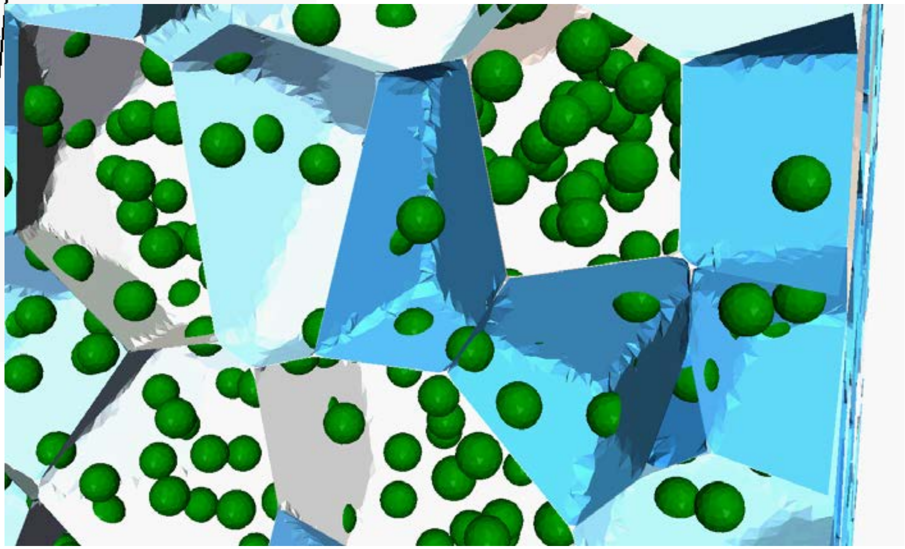
Zener Pinning





Zenner Pinning in 3D





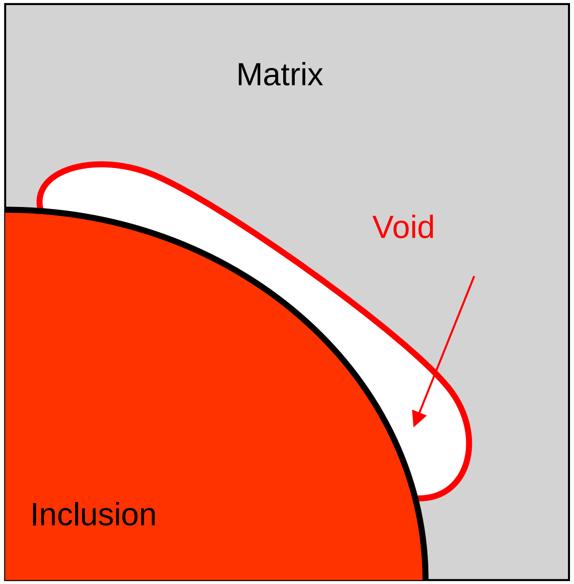
Particles and voids representation

➢ Level set functions

- 3 domains defined by $\alpha_i \quad \alpha_m \quad \alpha_v$

- Interfaces matrix – inclusions – voids: zero values of level-set functions

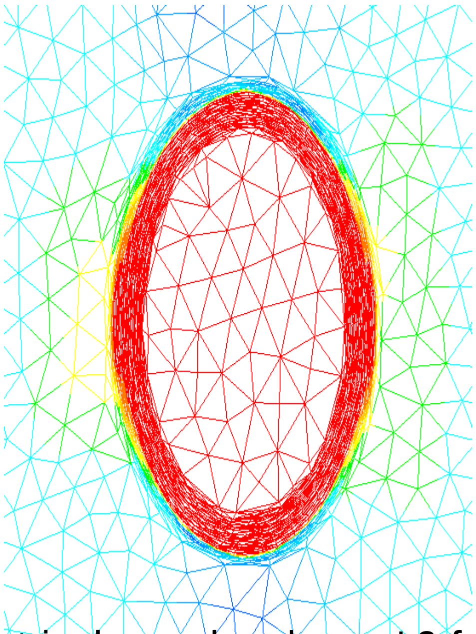
$$\begin{cases} x \in Inclusion \Leftrightarrow \alpha_i(x) \geq 0 \\ x \in Matrix \Leftrightarrow \alpha_m(x) \geq 0 \\ x \in Void \Leftrightarrow \alpha_v(x) = -\max(\alpha_i(x), \alpha_m(x)) \geq 0 \end{cases}$$



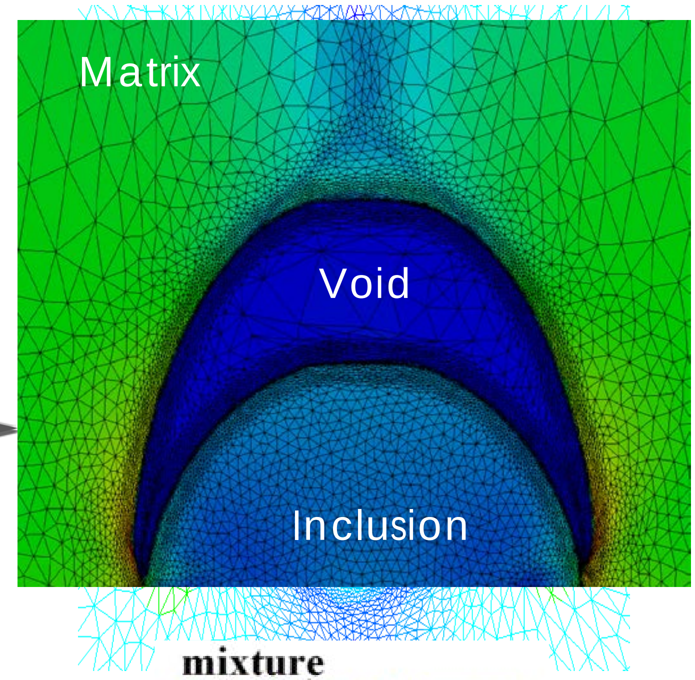
[Roux et al., *Computational Materials Science*, 2013]

Particles and voids representation

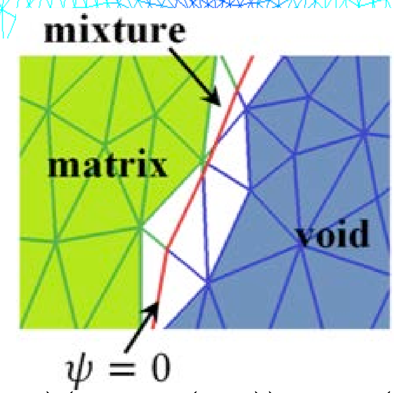
Anisotropic mesh adaptation



Mesh adaptation
Metrics mixing



Metric based only on LS function

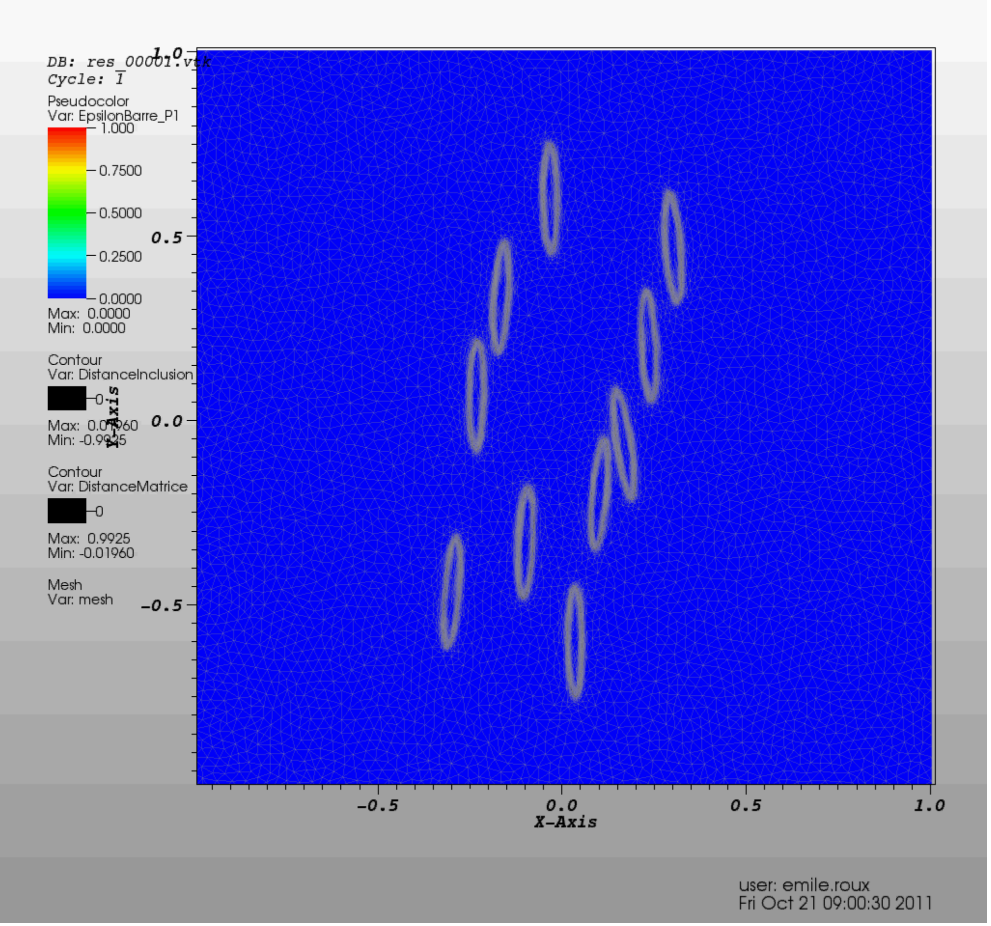


- **Mechanical properties**
  - Each domain has its own mechanical properties
  - Implicit description of interfaces
    - ➠ Some elements are crossed by interfaces
    - ➠ Linear mixing of mechanical properties

$$P_{mat} = \left(\varphi_v(\alpha_v)P_v + \left(1-\varphi_v(\alpha_v)\right)P_i\right)\left(1-\varphi_m(\alpha_m)\right) + \varphi_m(\alpha_m)P_m$$

[Roux et al., *Computational Materials Science*, 2013]

Nucleation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Cycle: 1
Pseudocolor
Var: EpsilonBarre_P1
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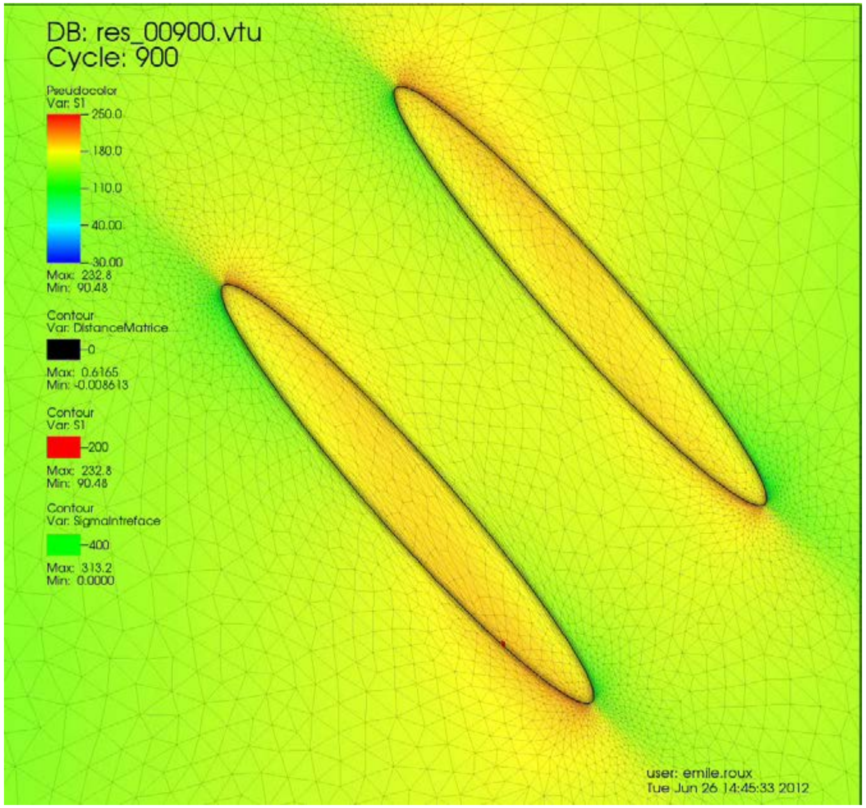
0.7500
0.5000
0.2500
0.0000
Max: 0.0000
Min: 0.0000
Contour
Var: DistanceInclusion
0
Contour
Var: DistanceMatrice
0
Max: 0.9925
Min: -0.01960
Mesh
Var: mesh
1.0
0.5
0.0
-0.5
Y-Axis
-0.5
0.0
0.5
1.0
X-Axis
user: emile.roux
Fri Oct 21 09:00:30 2011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Pseudocolor
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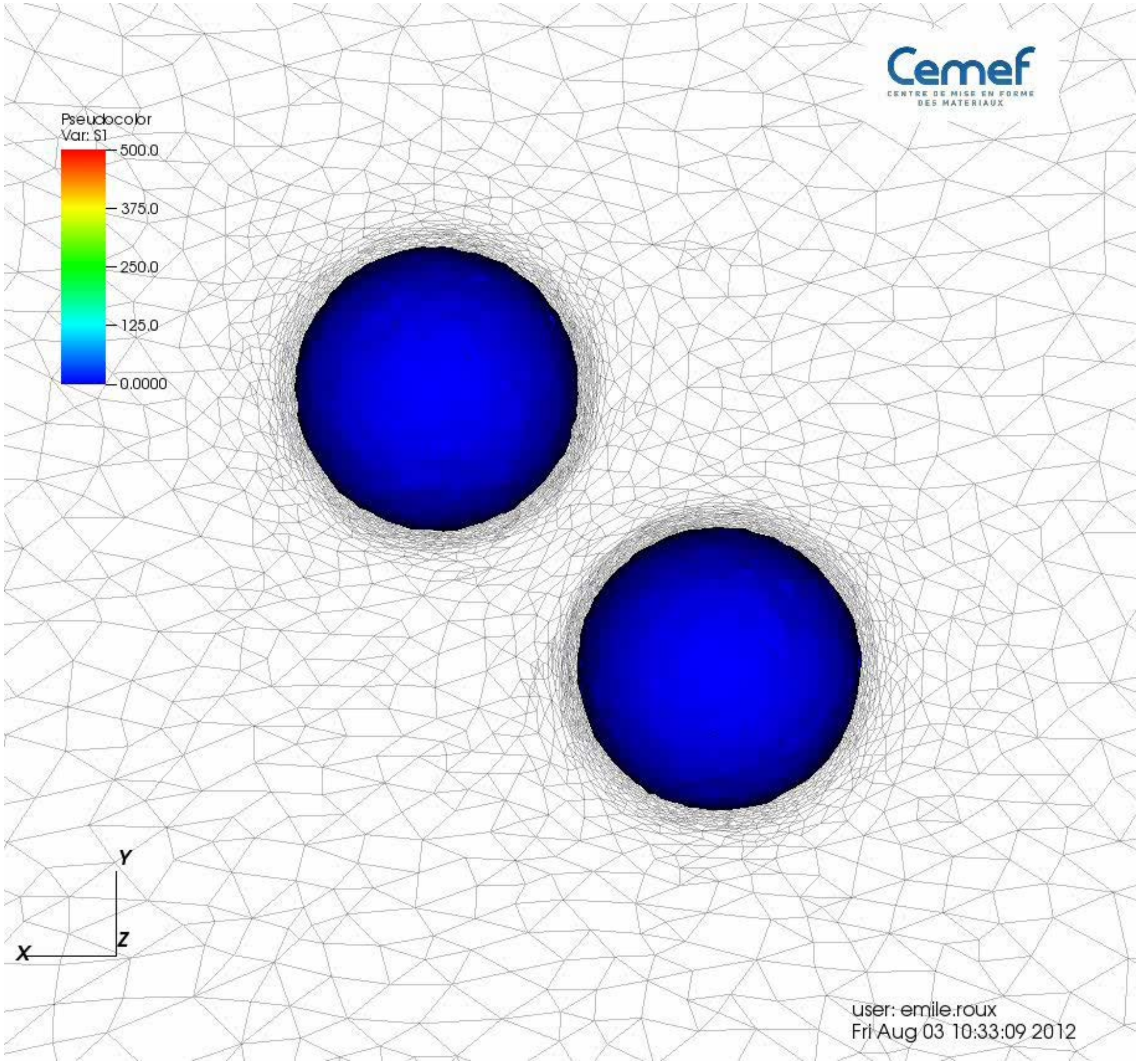
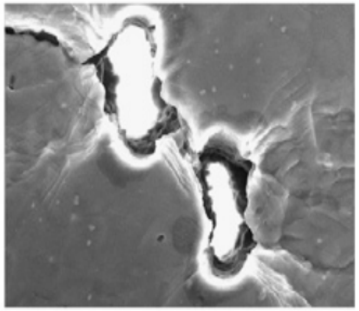
250.0
180.0
110.0
40.00
-30.00
Max: 232.8
Min: 90.48
Contour
Var: DistanceMatrice
0
Max: 0.6165
Min: -0.008613
Contour
Var: S1
200
Max: 232.8
Min: 90.48
Contour
Var: SigmaInterface
400
Max: 313.2
Min: 0.0000
user: emile.roux
Tue Jun 26 14:45:33 2012

Multiscale analysis of failure

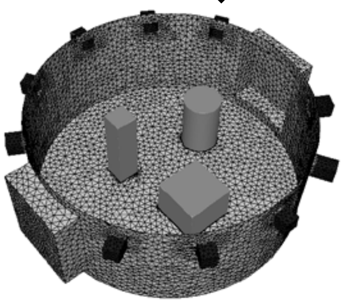
- Ductile failure modeling at the microscale: nucleation, growth & coalescence

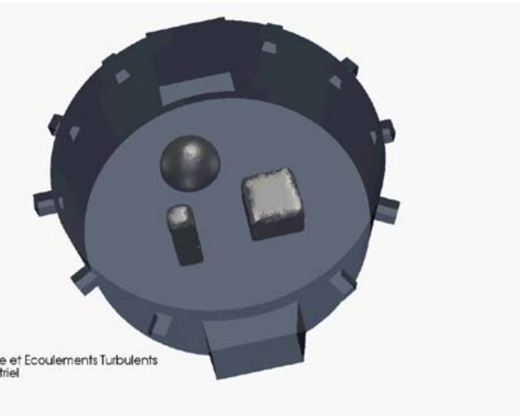




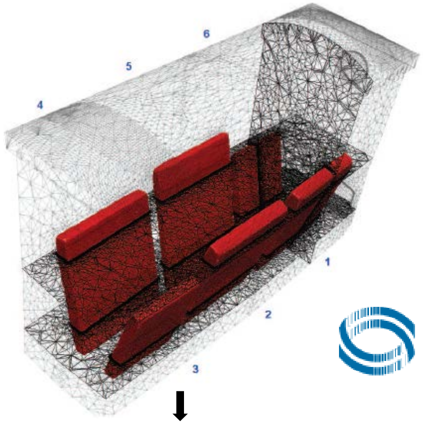
Application to conjugate heat transfer

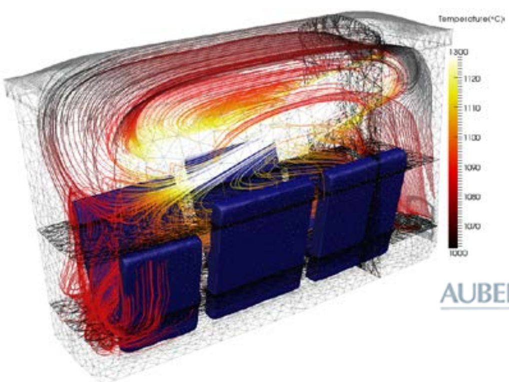
Aubert & Duval



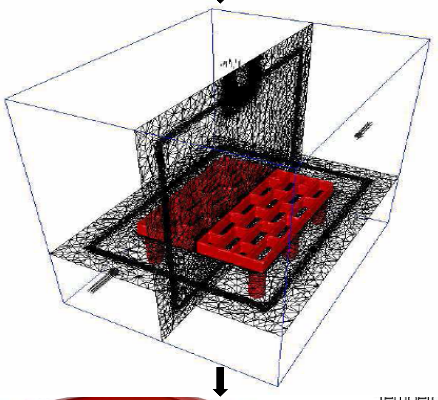


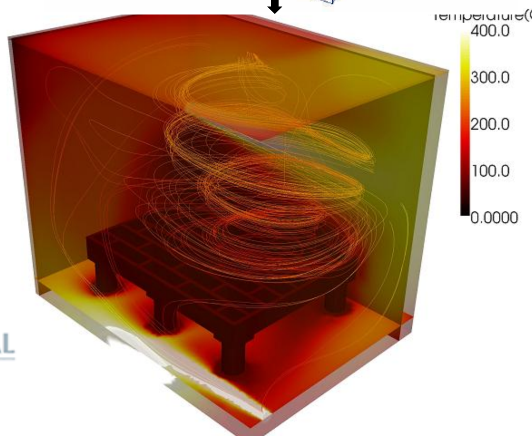
Industeel





Terreal





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SCIENCES COMPUTERS CONSULTANTS

AREVA

ArcelorMittal

Industeel

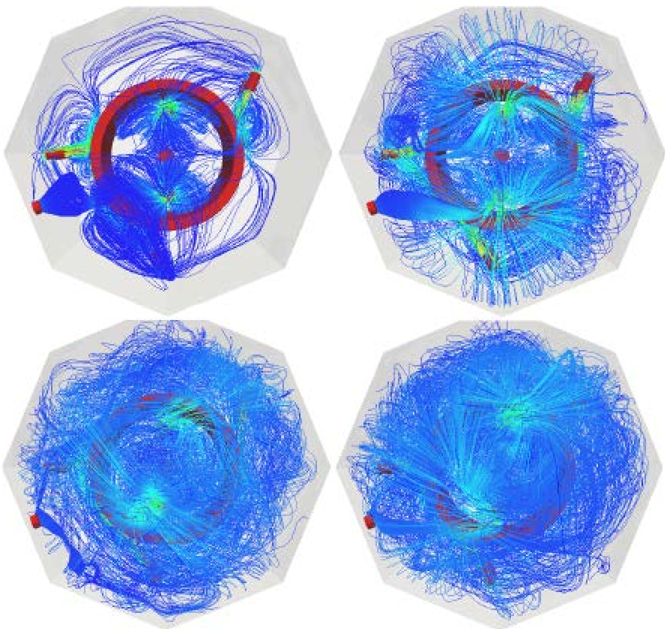
ANR
Programme Cosinus 2010

Snecma
Groupe SAFRAN

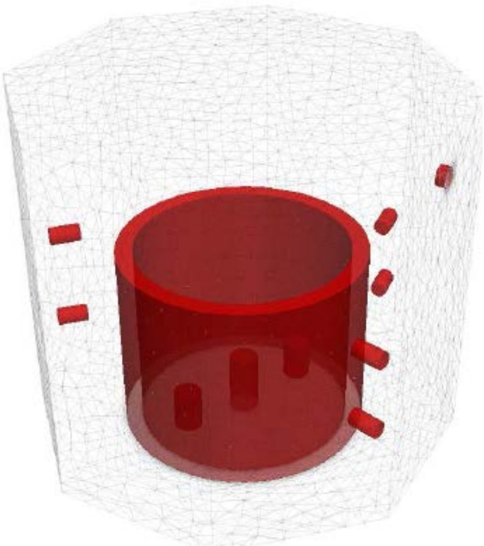
AUBERT&DUVAL

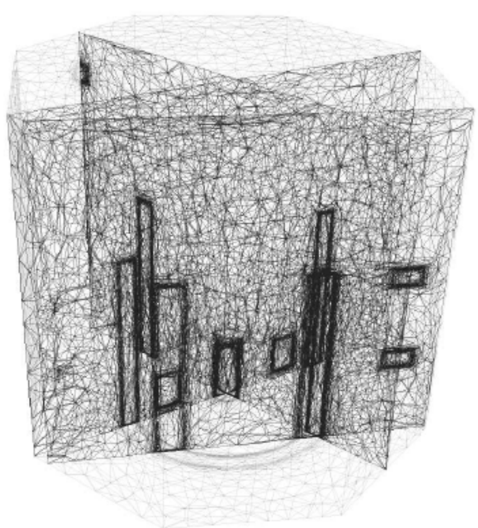
Multiphase flows

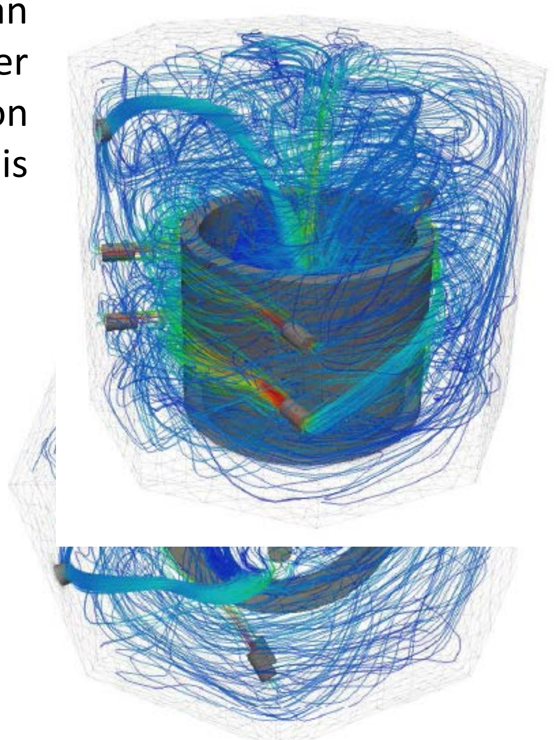
- Quenching process
- Turbulent boiling
- Phase change
- Vapor film bubbles growth and expansion
- surface tension



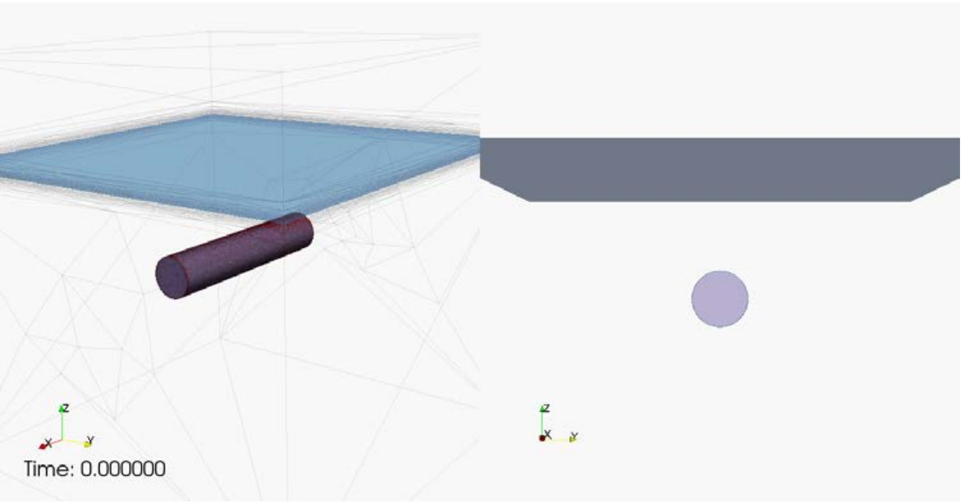
3D quenching of an ingot inside a water tank with agitation (no phase change is considered)

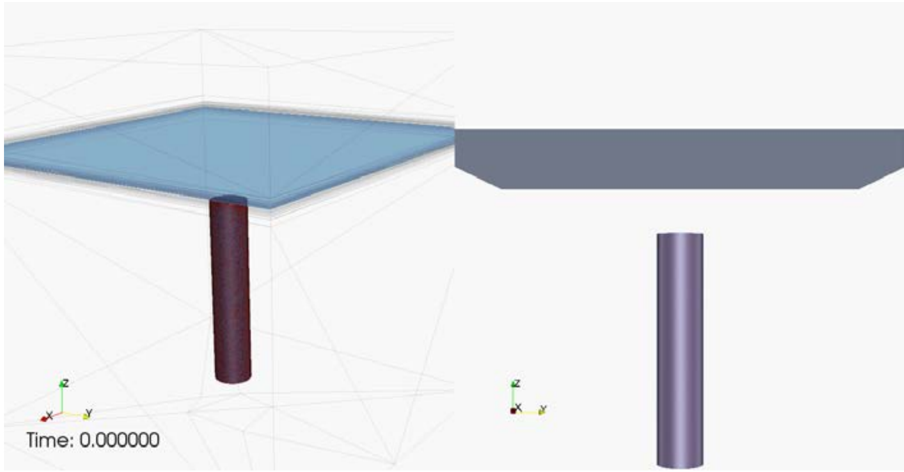


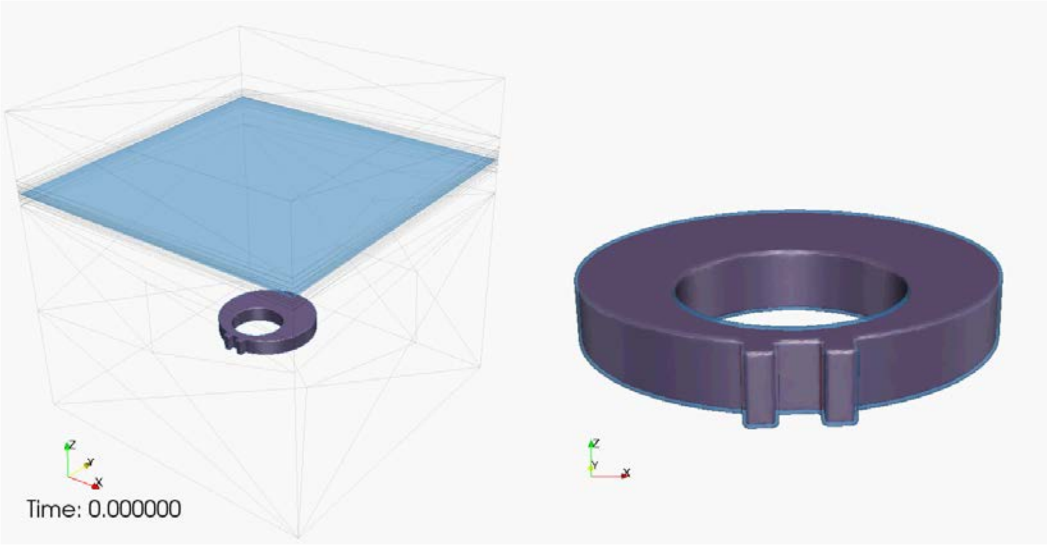




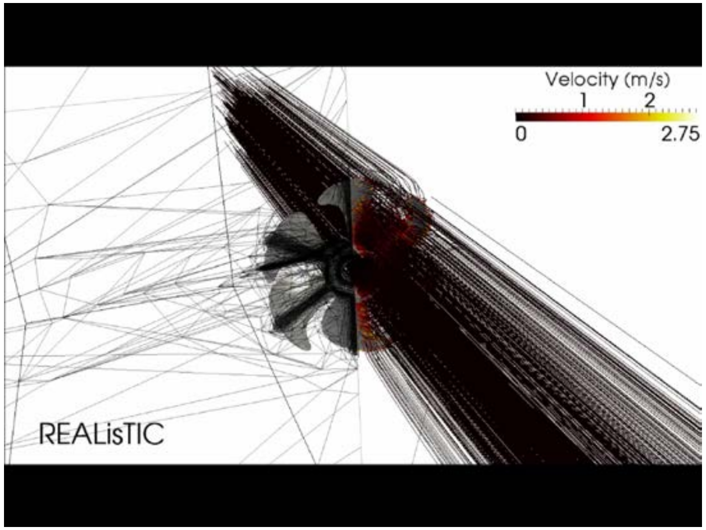
The direct simulation of boiling and turbulent vapor films generated from a heated solid inside a water tank

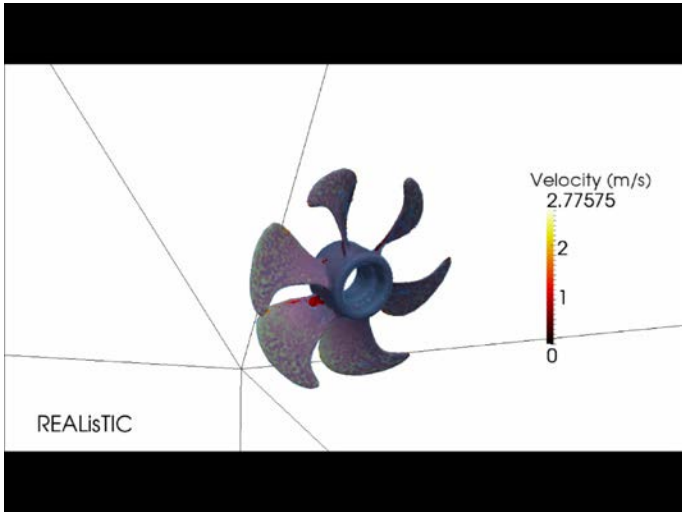


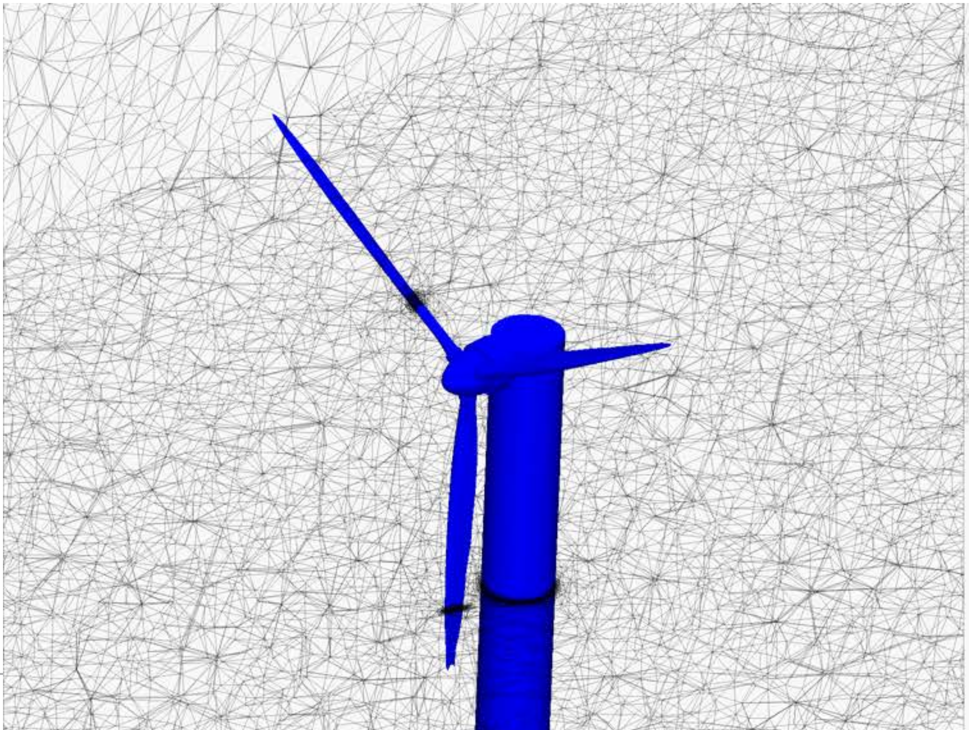


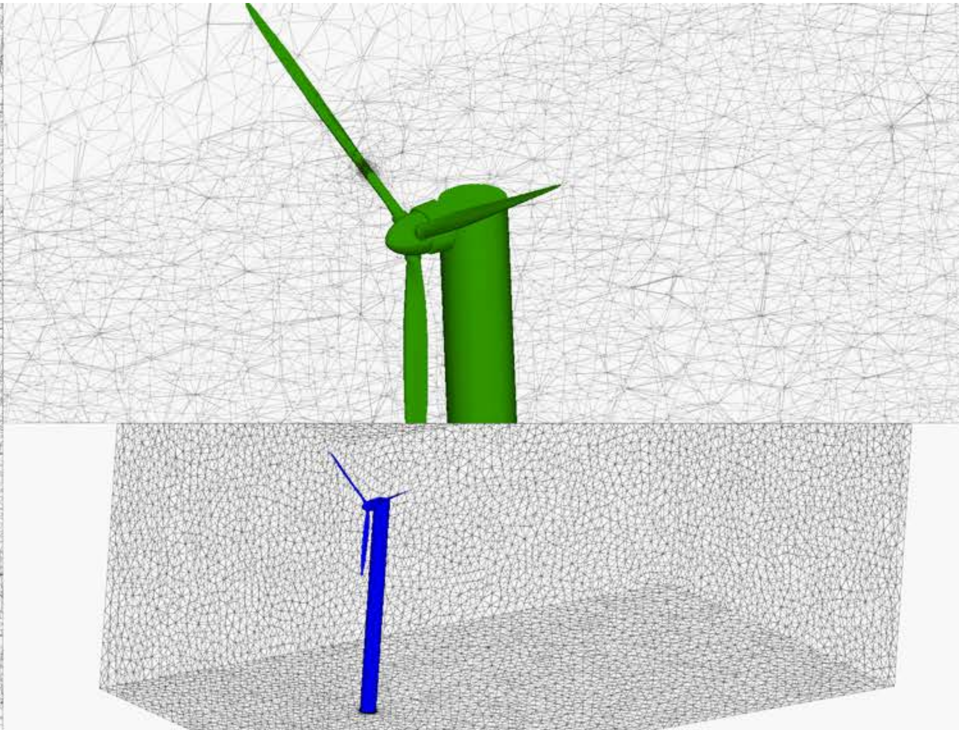


Application to moving structures

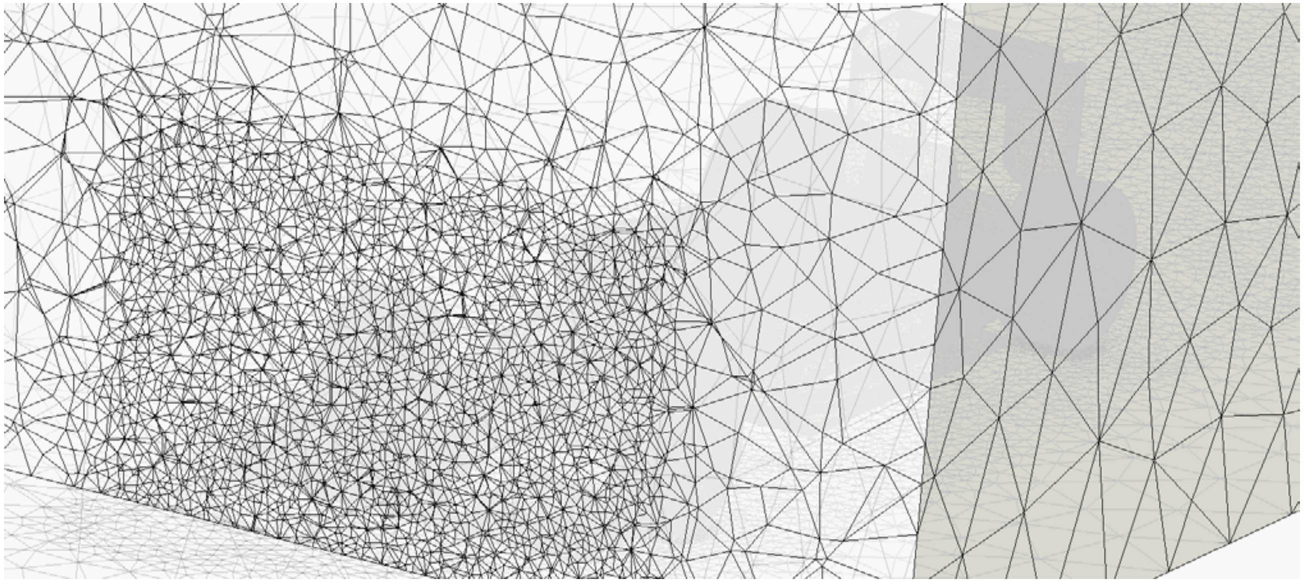




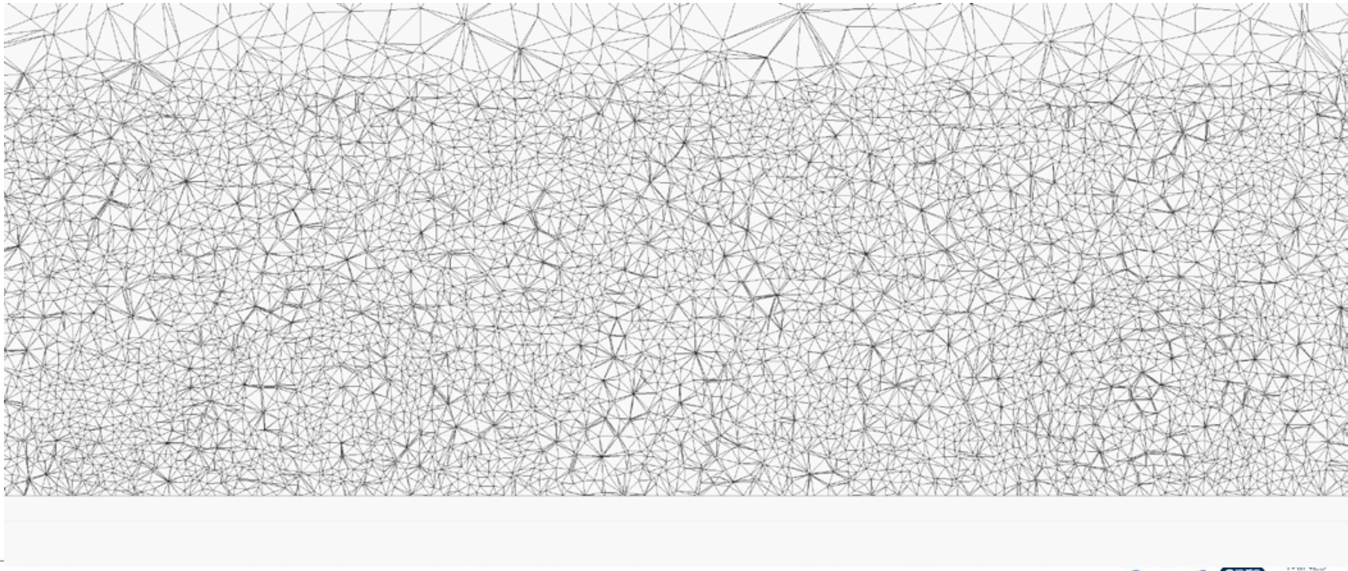




Towards extreme mesh adaptation for boundary layers problems



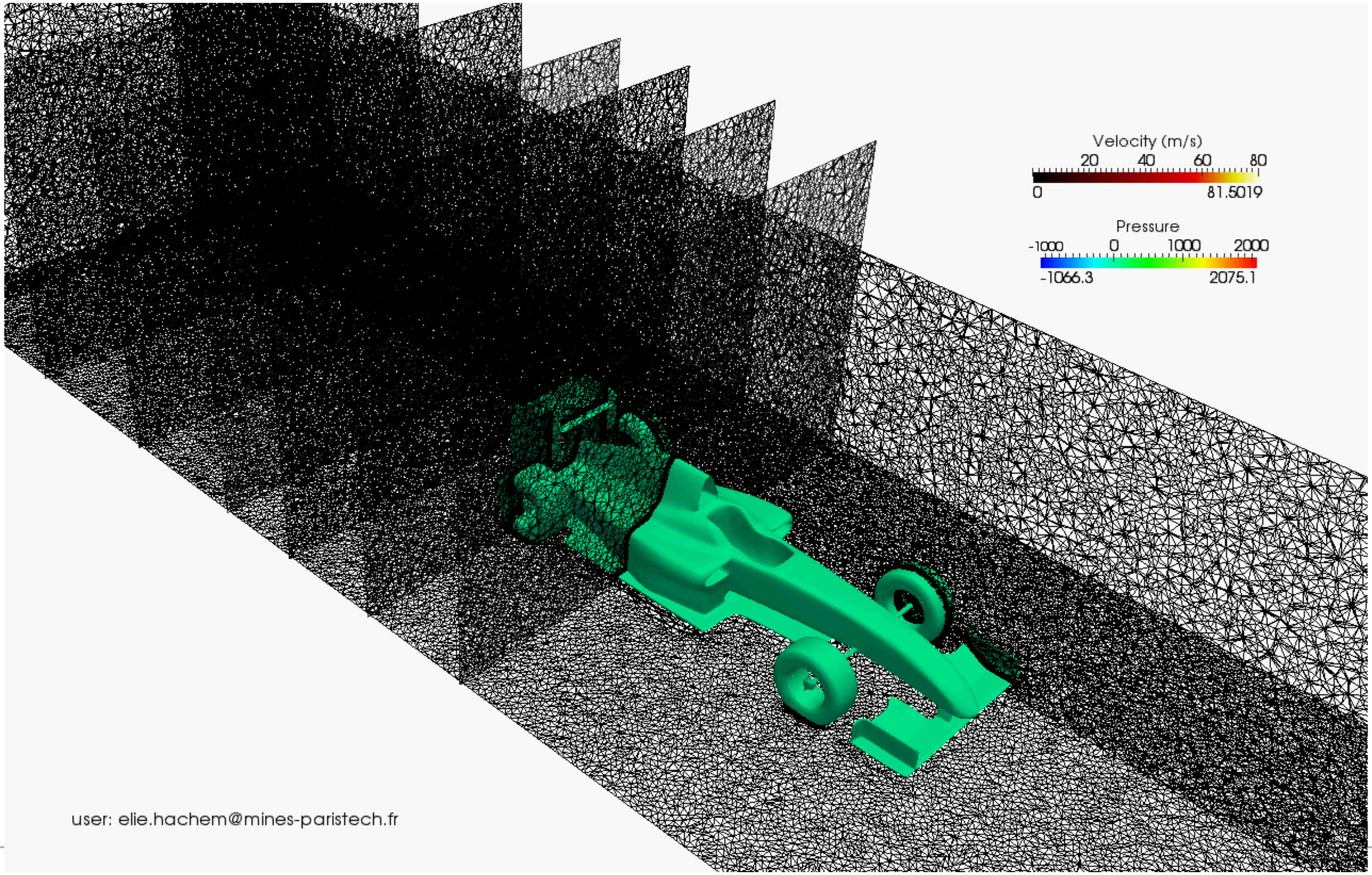
Combining:
- Immersed volume method
- Anisotropic meshing
- Parallel adaptation
- Boundary layers capturing



[E. Hachem, Y. Mesri, 2015]

Dynamic Anisotropic Mesh Adaptation

- Velocity: 300km/h
- Number of nodes: 2 millions
- Numer of cores: 96



Concluding Remarks

- ❑ Material forming simulation ➔ need to know the origin of the material and know where it goes
  - ✓ Forming including microstructure evolution
  - ✓ Heat Treatment ➔ Heating, Induction heating, quenching
  - ✓ In use-properties ➔ Damage prediction

- ❑ Development of numerical approaches
  - ✓ FE approach
  - ✓ Immersed domain + Level set interface➔ easy to represent different moving objects, great interest for **multi-scale and multi-physics approach**
  - ✓ Computational Time and Space Reduction
  - ✓ High Performance Computing

Performance of CIMLIB Library

- ✓ **Acces to the PRACE supercomputers**:
  - Curie (80 000 cores)
  - JuQUEEN (400 000 cores)
- ✓ **Run CimLib on a huge number of cores**:
  - 65 536 on Curie
  - 262 144 on JuQUEEN
- ✓ **Solve a 100 billion unknowns system**
  - 33,4 billion mesh nodes in 2D
  - 13,7 billion mesh nodes in 3D
- ✓ **NB : All computing toolchain should be parallel:**
  - Mesh generation to data analysis