

Méthode des champs de phase et homogénéisation numérique par transformées de Fourier : développements récents

A. Finel

Université Paris-Saclay, ONERA, CNRS, Laboratoire d'Etude des Microstructures, Châtillon, France



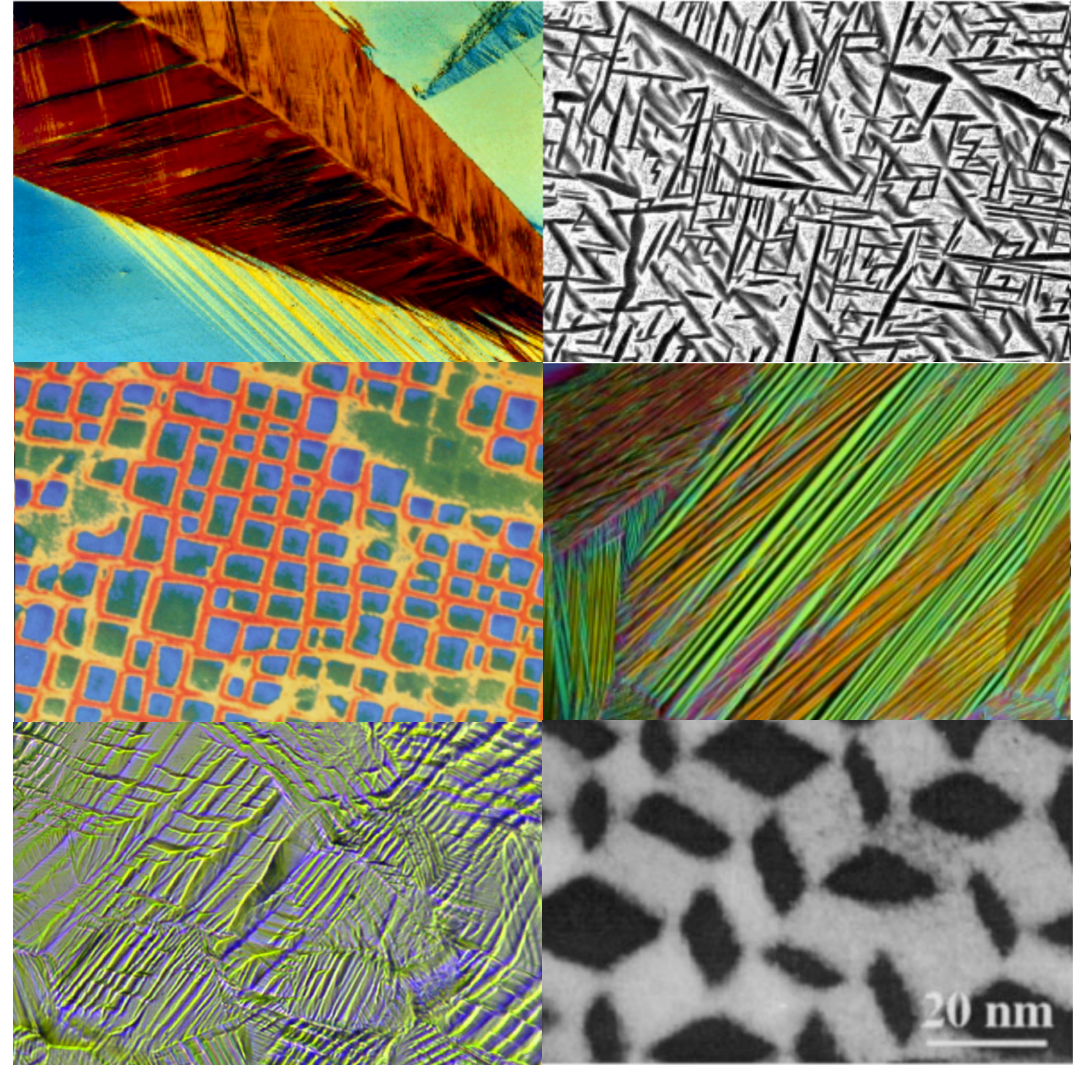
Contexte

Extremely diverse (and beautiful...) patterns :

- materials are always heterogeneous
- inherited from phase transformations during **elaboration**, or subsequent **thermo-mechanical** treatments
- microstructures can be detrimental or **beneficial** for **properties** (mechanical, magnetic, electrical...)
- comprehensive modelling of the relationships between microstructure and properties to **understand** material behaviour
- length scales (μm) $\gg$ atomic scale !!!

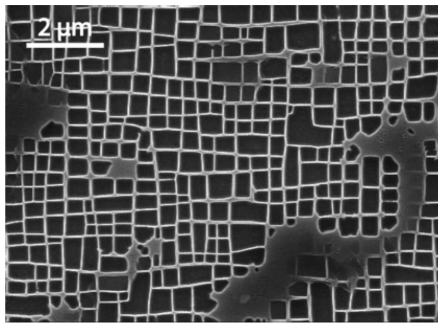
A mesoscopic (continuous) modelling is needed !

→ Phase Field method !

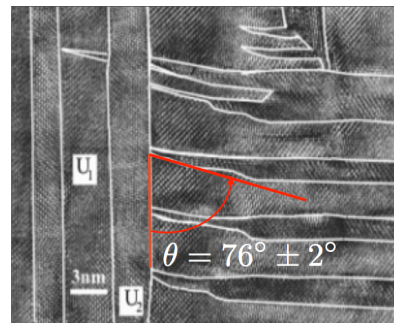


Phase Field Method : a few examples

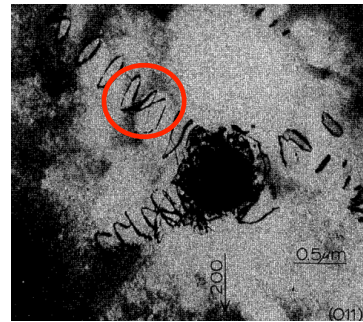
Ni-based
superalloys



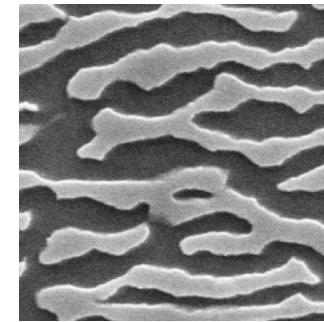
Shape memory
alloys



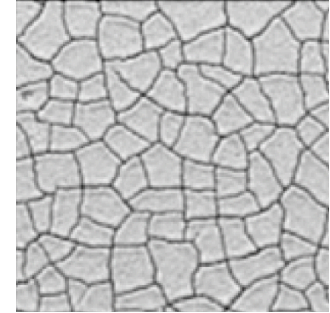
Coherency
loss



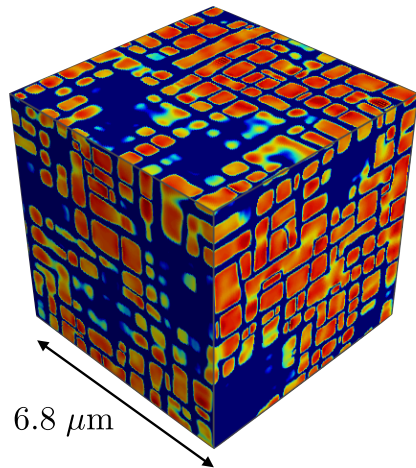
Rafts in Ni-based
superalloys



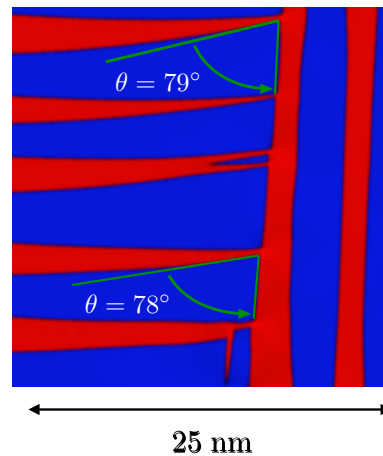
Cracks patterns
in thin films



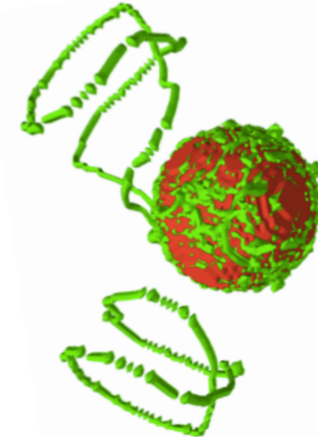
Cottura et al
Acta Mat. (2021)



Finel et al,
C. R. Phys. (2010)



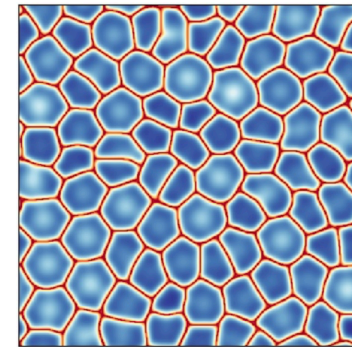
Geslin et al,
APL (2014)



Cottura et al,
(2026)



Degeiter et al,
(in preparation)

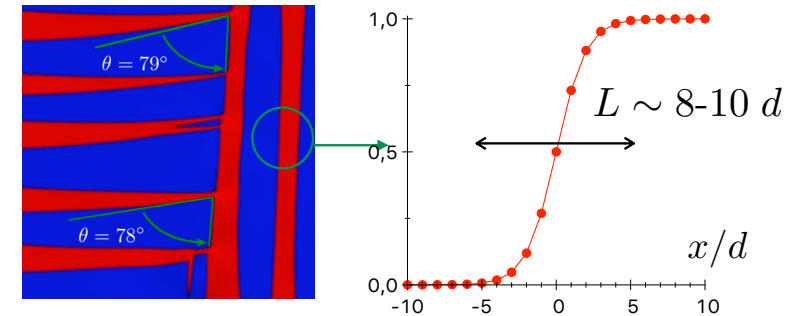


Challenges

1. Computational cost :

- continuous modelling (interfaces are diffuse) : no interface tracking
- but, we need a grid with a grid spacing small enough : $d \ll L$

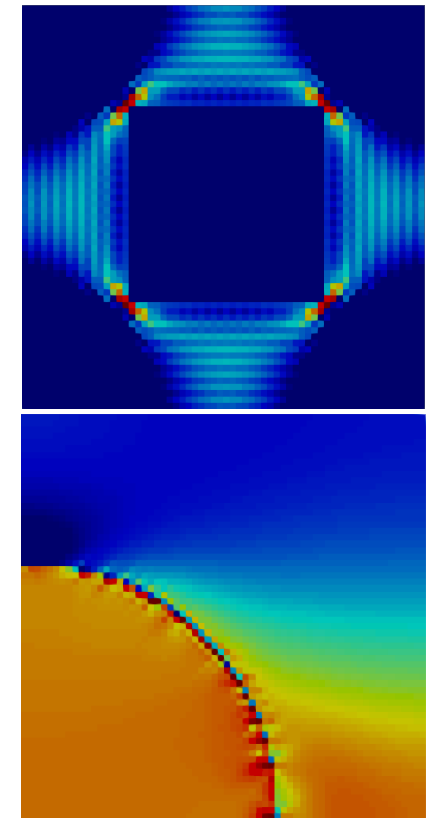
→ *how to write a PFM that permits to resolve interfaces with very few points ?*



2. Coupling with mechanical fields :

- microstructures contain internal elastic stresses
- FFT-based solver for mechanical equilibrium : easy to implement and fast (Khachaturyan 1995...; Moulinec-Suquet 1998...)
- but : formulations not adapted to sharp interfaces (Gibbs oscillations, slow convergence if high elastic contrast...)

→ *we need a “robust” FFT solver !*



3. FFT solvers are based on regular grids :

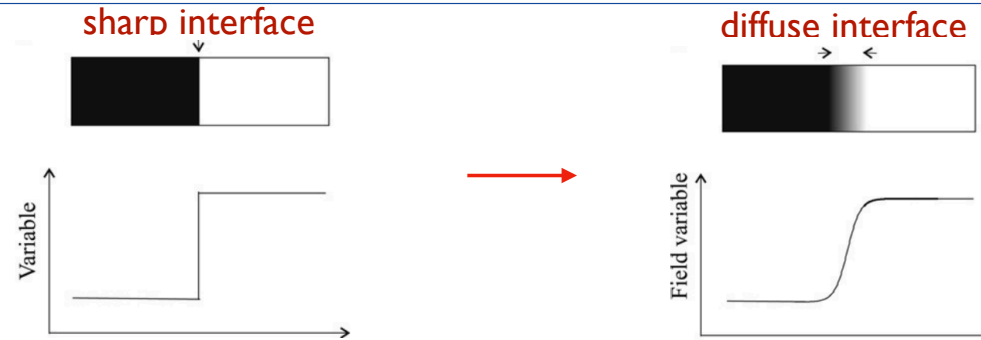
- interfaces are not conform to the grid
- local undesired (stress) fluctuations along the interfaces

→ *how to suppress these artefacts ?*

Outline

1. The Sharp Phase Field Method (S-PFM)
2. A robust FFT-based solver for microstructures with sharp interfaces
3. FFT-solvers on non-uniform grids (in progress...)

“Classical” Phase Field Method

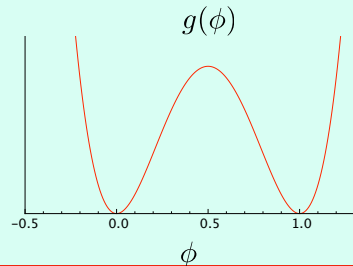


Continuous formulation :

$$F = \int d^3x \left\{ g(\phi) + \frac{1}{2} \lambda |\nabla \phi|^2 \right\}$$

$$g(\phi) = A \phi^2 (1 - \phi)^2$$

$$\frac{\partial \phi}{\partial t} = -L \frac{\delta F}{\delta \phi}$$

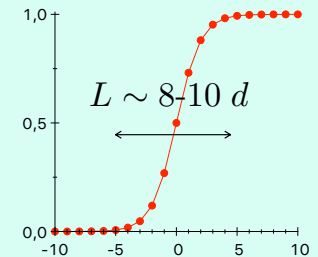


Equilibrium profile :

$$\phi^{eq} = \frac{1}{2} \left(1 + \tanh \left\{ \frac{2(x - x_0)}{l} \right\} \right)$$

interface thickness : $l = \sqrt{\frac{\lambda}{2 \Delta F}}$

Code → discrete grid, grid spacing d



→ diffuses interfaces :

- No pinning : grid spacing $d \ll$ interface thickness $l \rightarrow$ limitation on accessible linear dimension
- 3D simulations computationally intensive

→ what we want :

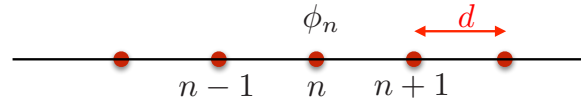
- A phase field method with interface thickness $l \ll d$
- Ideally : interface width reduced to only one grid point !

The Sharp Phase Field pour Method (S-PFM)

Finel et al, PRL (2018)

A discrete formulation !

Consider a 1D lattice :



Discrete free energy functional :

$$F = \sum_n \left\{ g(\phi_n) + \frac{\lambda}{2d^2} (\phi_{n+1} - \phi_n)^2 \right\}$$

Interface at equilibrium : $\frac{\delta F}{\delta \phi_n} = 0$

$$g'(\phi_n) - \frac{\lambda}{d^2} (\phi_{n+1} + \phi_{n-1} - 2\phi_n) = 0 \quad \text{Eq. I}$$

→ Question :

$\exists? g(\phi)$ such that, if $\phi_n = f(nd)$ is the equilibrium profil, $f(nd - x_0)$ is also an equilibrium profil $\forall x_0 \in \mathbb{R}$?

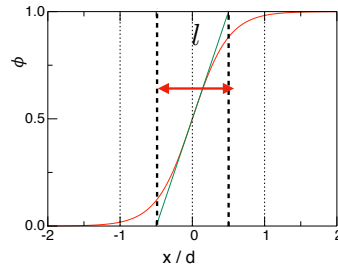
→ Procedure :

• look for a function $f(x)$ such that, if $\phi_n = f(nd - x_0)$, $(\phi_{n+1} + \phi_{n-1} - 2\phi_n)$ is function of ϕ_n independent of x_0 !!!

• i.e. look for a function $f(x)$ such that, if $\phi_n = f(nd - x_0)$, Eq. I becomes an ODE independent of x_0 !!!

→ Choice : • select any interface thickness : l , even with $l < d$

$$f(x) = \frac{1}{2} \left(1 + \tanh \frac{2x}{l} \right)$$



$$\text{Then : } 2\phi_{n\pm 1} - 1 = \frac{(2\phi_n - 1) \pm \alpha}{1 \pm (2\phi_n - 1)\alpha}$$

$$\alpha = \tanh\left(\frac{2d}{l}\right)$$

Eq. I :

$$g'(\phi) = \frac{\lambda}{d^2} \left\{ \frac{1 - \alpha^2}{1 - \alpha^2(2\phi - 1)^2} - 1 \right\} (2\phi - 1)$$

Solution :

$$g(\phi) = \frac{\lambda}{4d^2} \left\{ \frac{\alpha^2 - 1}{\alpha^2} \log[1 - \alpha^2(1 - 2\phi)^2] - (1 - 2\phi)^2 \right\}$$

The Sharp Phase Field pour Method (S-PFM)

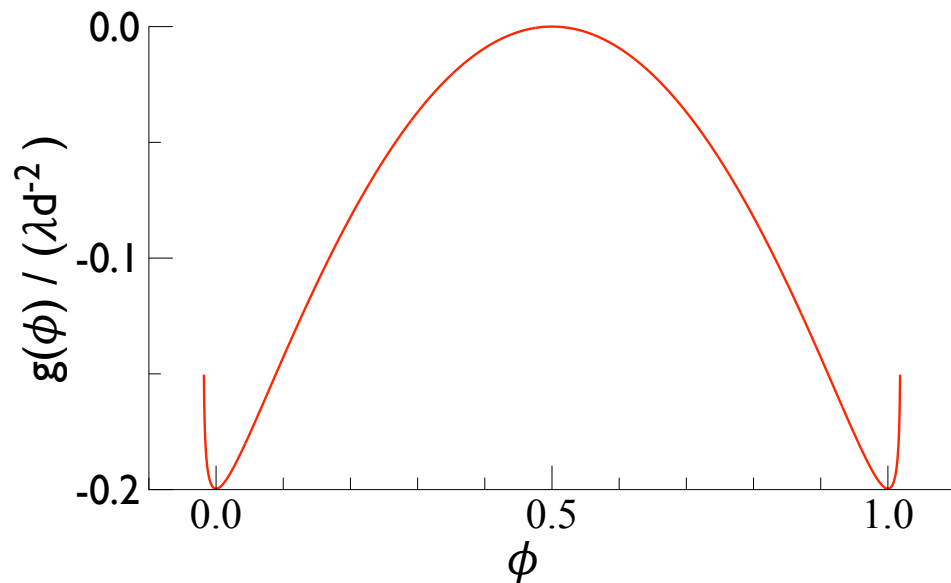
free energy density

$$g(\phi) = \frac{\lambda}{4d^2} \left\{ \frac{\alpha^2 - 1}{\alpha^2} \log[1 - \alpha^2(1 - 2\phi)^2] - (1 - 2\phi)^2 \right\}$$

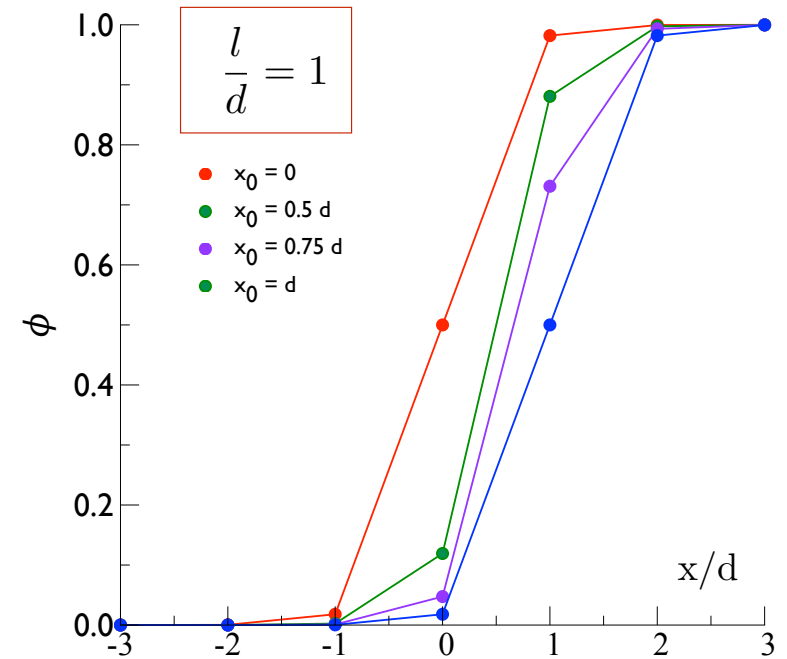
$$\alpha = \tanh\left(\frac{2d}{l}\right)$$

→ Exemple :

$$\frac{l}{d} = 1$$



no pinning even for sharp interfaces



→ same interface energy (10^{-14}): $\sigma_{int} \simeq 0.44263 \lambda d^{-1}$

→ interface energy is exactly invariante by translation !

S-PFM in 3D

Extension to 3D : need to recover rotational invariance

- extend gradient terms to n^{th} neighbours, with weighting coefficients γ_i selected to recover rotational invariance:

C

$$F = \sum_{\vec{r}} \{ g(\phi(\vec{r})) + \frac{\lambda}{2} \sum_{i=1}^n \gamma_i \frac{\nu_i}{d_i^2} \sum_{k=1}^{m_i} \|\phi(\vec{r} + \vec{r}_i(k)) - \phi(\vec{r})\|^2 \}$$

$$\sum_{i=1}^n \gamma_i = 1$$

$$g(\phi) = \frac{\lambda}{4} \sum_{i=1}^3 \gamma_i \frac{\nu_i}{d_i^2} \sum_{k=1}^{m_i} \left\{ \frac{\alpha_i(\vec{r}_i(k))^2 - 1}{\alpha_i(\vec{r}_i(k))^2} \log[1 - \alpha_i(\vec{r}_i(k))^2 (2\phi - 1)^2] - (2\phi - 1)^2 \right\}$$

$\vec{u}$: unitary vector perpendicular to planes $(h_1 k_1 k_1)$

Kinetics :

$$\frac{\partial \phi}{\partial t} = -L \frac{\delta F}{\delta \phi}$$

Quality of the S-PFM

growth of a single precipitate

free energy density

$$g_{tot}(\phi) = g(\phi) - \Delta F h(\phi)$$

kinetics

$$\frac{\partial \phi}{\partial t} = -L \frac{\delta F}{\delta \phi} = -L \left\{ g'_{tot}(\phi) - \frac{\lambda}{d^2} \tilde{\nabla}^2 \phi \right\}$$

$$\Delta F > 0$$

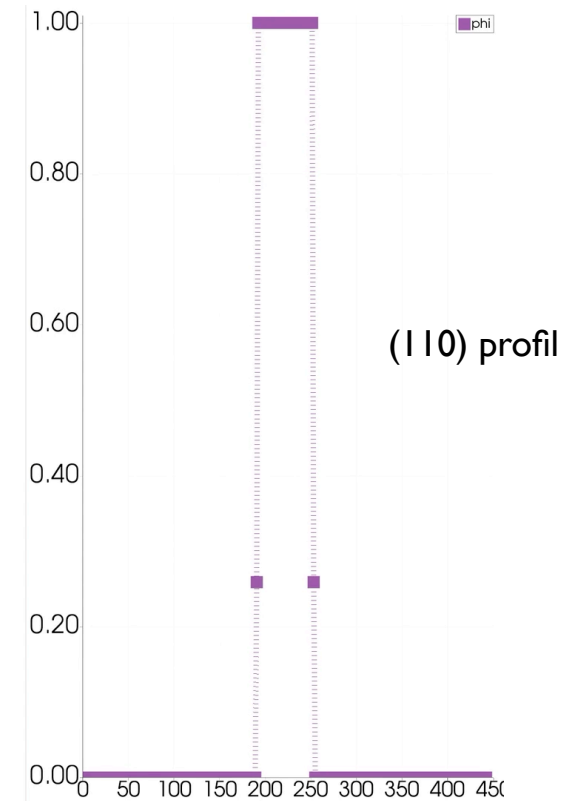
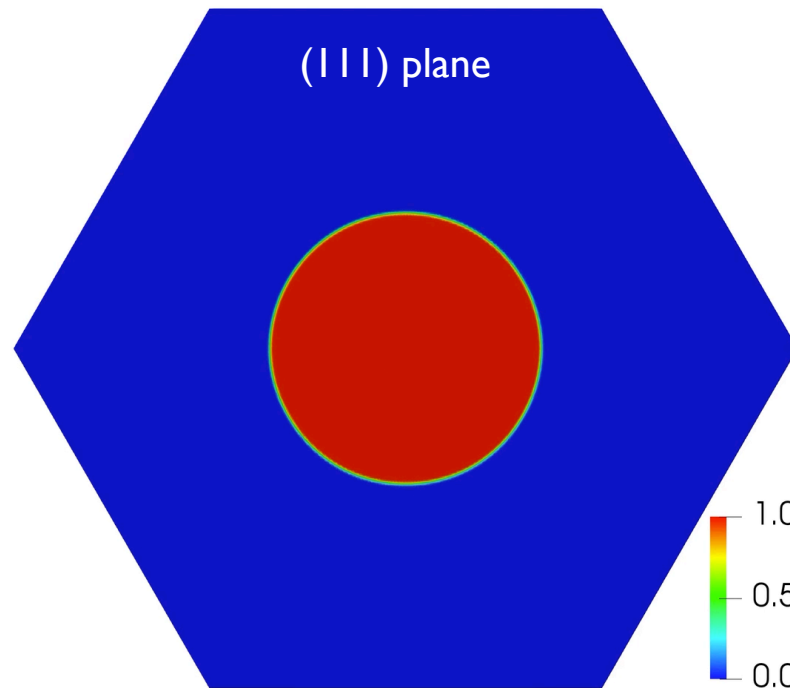
$$h(\phi) = 3\phi^2 - 2\phi^3$$

$$\text{precipitate : } \phi = 1$$

$$\text{matrice : } \phi = 0$$

simulation : 256x256x256

$$\frac{l}{d} = \frac{2}{3}$$

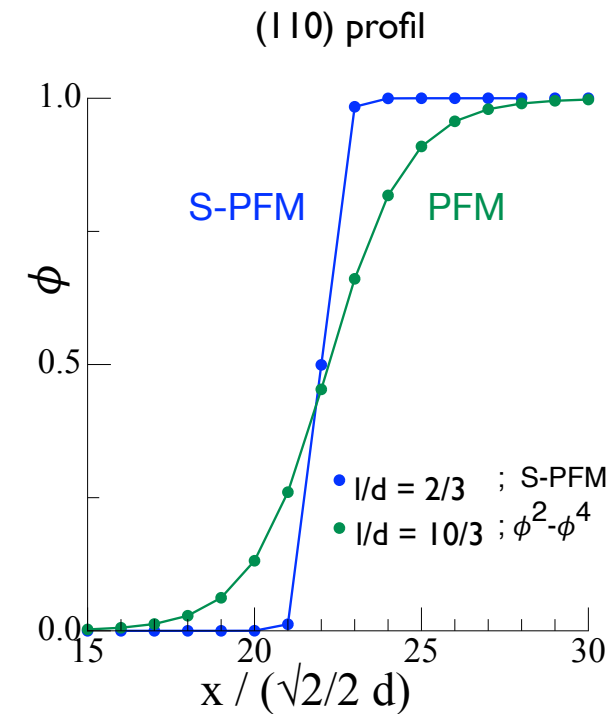
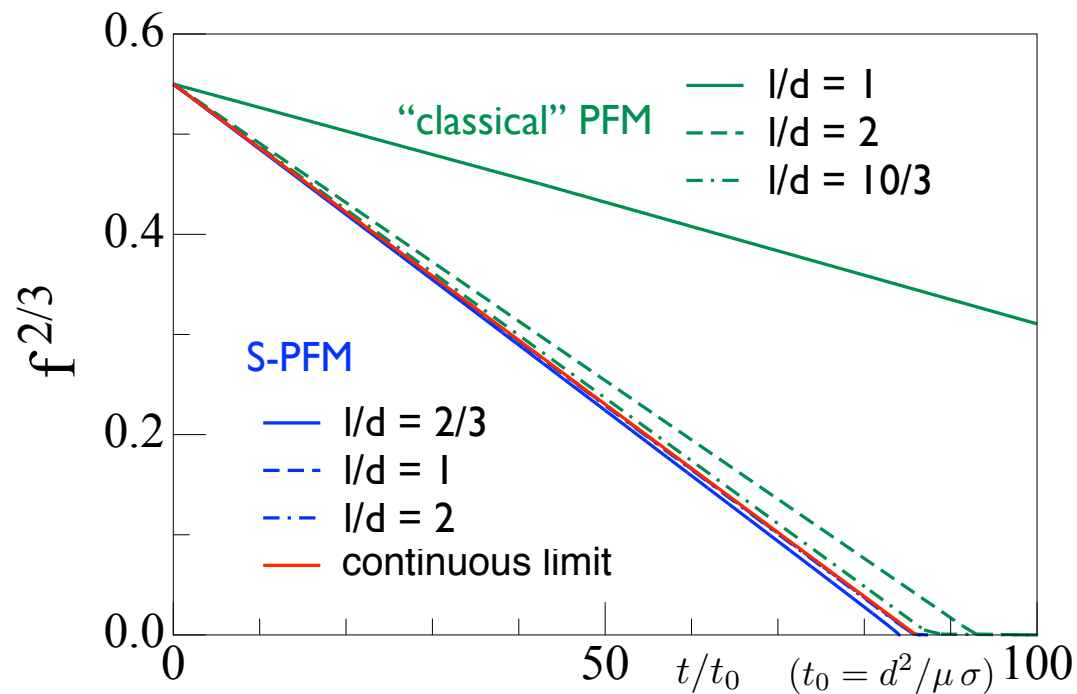


Interfacial kinetic properties

ability of S-PFM to reproduce the “exact” interfacial kinetics

Curvature-driven collapse of a single precipitate :

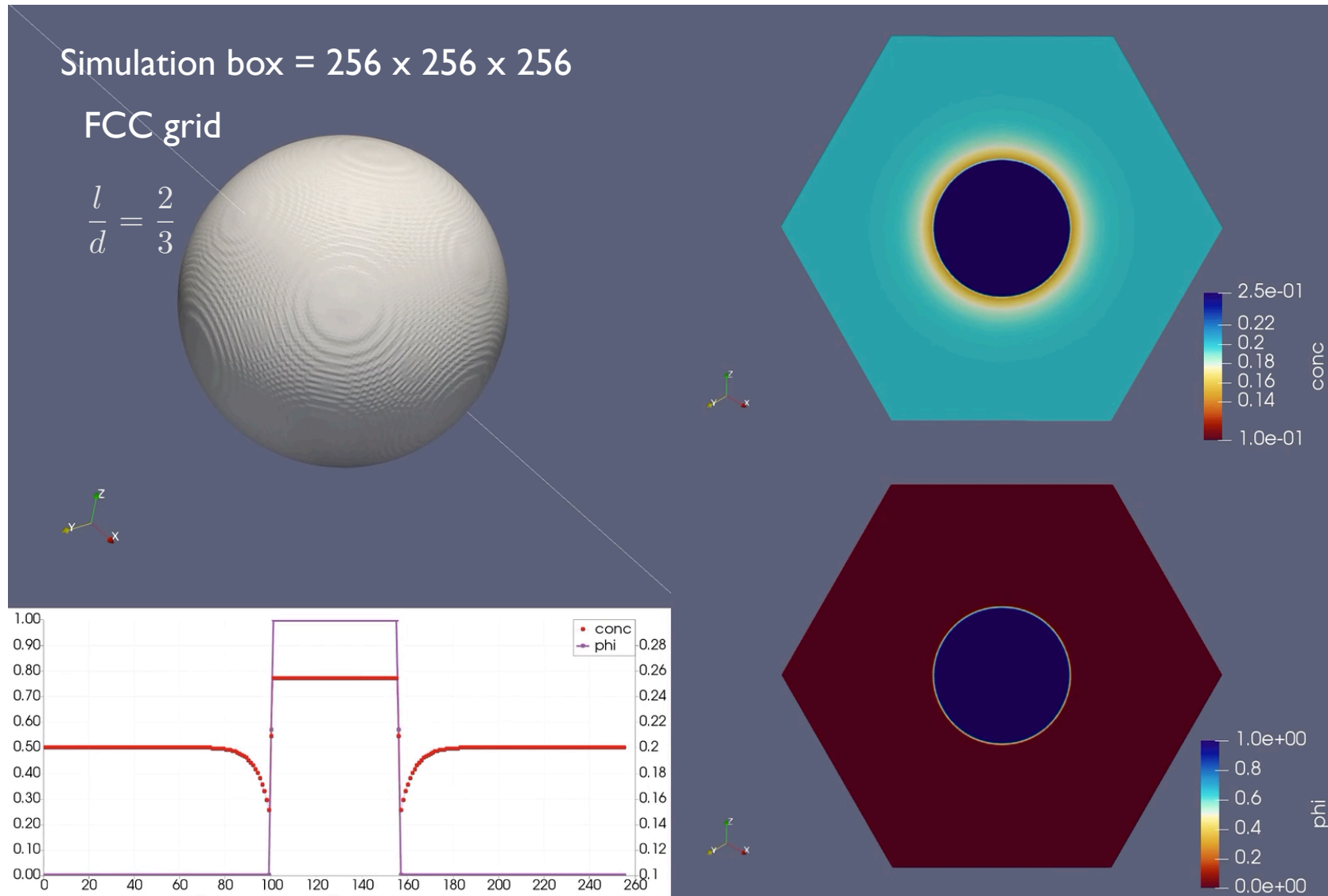
→ comparison S-PFM / “classical” PFM :



→ For a precision on the interface velocity of env. 1.7% :

S-PFM : $l/d = 2/3$	→	1 grid point in the interface
“classical” PFM : $l/d = 10/3$	→	8 grid points in the interface

S-PFM with a conserved order parameter



S-PFM with a conserved order parameter and elastic fields

 Inhomogeneous elasticity :

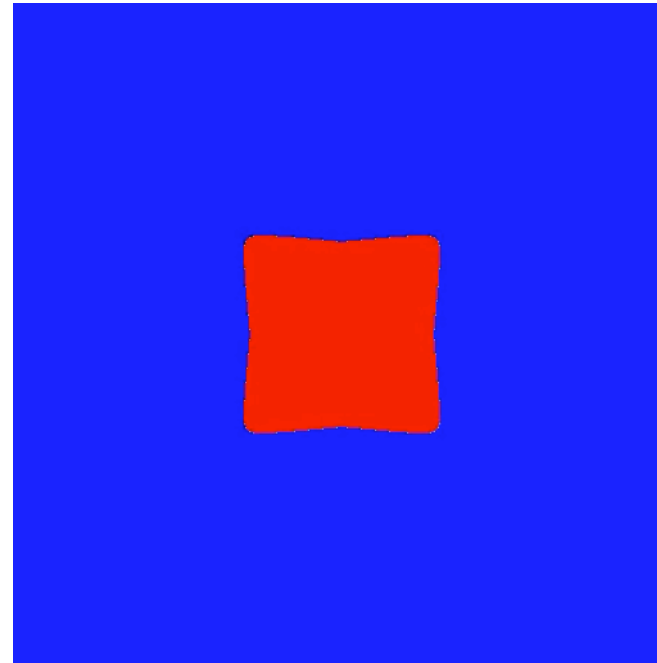
$$\gamma \quad \begin{array}{l} C_{11} = 197 \text{ GPa} \\ C_{12} = 144 \text{ GPa} \\ C_{44} = 90 \text{ GPa} \end{array}$$

$$\gamma' \quad \begin{array}{l} C_{11} = 193 \text{ GPa} \\ C_{12} = 113 \text{ GPa} \\ C_{44} = 132 \text{ GPa} \end{array}$$

concentration field



phase field



$$\frac{l}{d} = 1$$

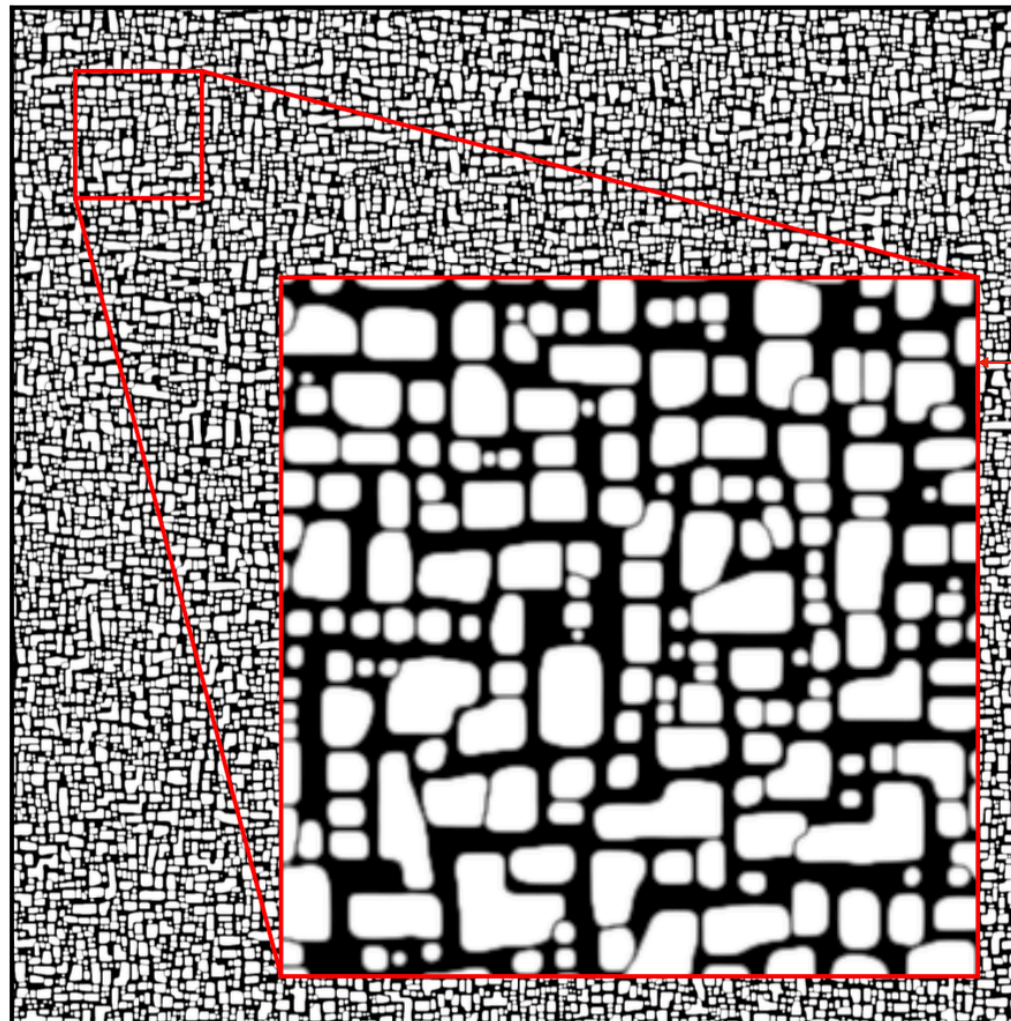
S-PFM : an application

Degeiter M., PhD (2019)

Microstructures in a
Ni-based super-alloy

S-PFM

2048x2048



"classical"

2048x2048

Outline

1. The Sharp Phase Field Method (S-PFM)
- 2. A robust FFT-based solver for microstructures with sharp interfaces**
3. FFT-solvers on non-uniform grids (in progress...)

Context

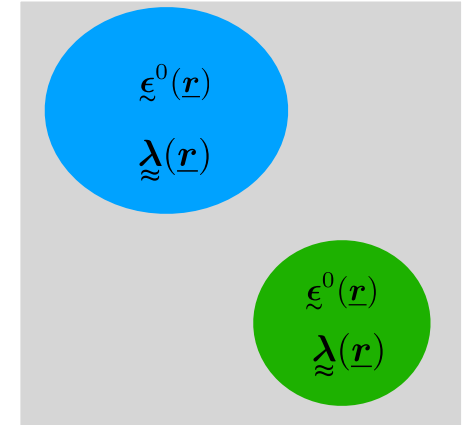
Fourier-based solver :

- microstructure : $\underline{\epsilon}^0(\underline{r})$ and $\underline{\lambda}(\underline{r})$
- mechanical equilibrium : $\underline{\sigma}(\underline{r}) = \underline{\lambda}(\underline{r}) : (\underline{\epsilon}(\underline{r}) - \underline{\epsilon}^0(\underline{r}))$ $\text{div } \underline{\sigma}(\underline{r}) = 0$
- “classical” Fourier-based solver : Khachaturyan (1995), Moulinec-Suquet (1994, 1998)

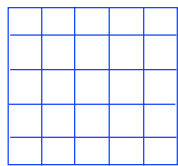
$$\frac{\partial}{\partial \underline{r}} \phi(\underline{r}) \xrightarrow{\text{FT}} i \underline{q} \phi(\underline{q})$$



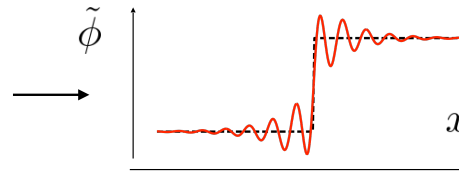
sharp interfaces need $|\underline{q}| \rightarrow \infty$



- numerics :



$$|\underline{q}| < Q_{max} \approx \frac{\pi}{d}$$



- overshoot near discontinuities $\forall d$! (Gibbs phenomenon)
- oscillations of period $2d$ (Nyquist frequency)
- convergence problem if high elastic contrast (cracks, voids...)

→ need “discrete” FFT-based solvers :

- able to handle sharp interfaces (high material contrasts in elastic stiffness, eigenstrain...)
- that generates no artefacts (Gibbs oscillations, overshoot...) due to High Frequency cut-off generated by the discrete grid
- that converges for any contrast (even ∞)
- and fast (convergence rate) !

FFT-based solvers : discrete formulation

Choice of a stencil :

- discrete grids for displacement $\underline{u}(\underline{r})$ and strain $\underline{\epsilon}(\underline{r})$
- replace derivatives by finite differences :

→ ex : centered scheme :

$$\epsilon_{11}(l, m, n) = \frac{1}{2} \{u_1(l+1, m, n) - u_1(l-1, m, n)\}$$

Discrete Fourier transforms :

$$\text{DFT} : \underline{u}(\underline{q}) = \frac{1}{N} \sum_{\underline{r}=(l,m,n)} \underline{u}(\underline{r}) \exp(-i\underline{q} \cdot \underline{r})$$

$$\epsilon_{11}(\underline{q}) = \frac{1}{2} (e^{iq_1} - e^{-iq_1}) u_1(\underline{q})$$

$$\rightarrow \underline{\epsilon}(\underline{q}) = \underline{D}(\underline{q}) \otimes_s \underline{u}(\underline{q}) \quad \text{with} \quad D_k(\underline{q}) = \frac{1}{2} (e^{iq_k} - e^{-iq_k}) = i \sin(q_k) \quad k = 1, 2, 3$$

Equilibrium in q-space :

$$\underline{\sigma}(\underline{r}) = \underline{\lambda}(\underline{r}) : (\underline{\epsilon}(\underline{r}) - \underline{\epsilon}^0(\underline{r}))$$

$$\text{Div } \underline{\sigma}(\underline{r}) = 0$$

Polarisation tensor

$$\underline{\tau}(\underline{q}) = \underline{\sigma}(\underline{q}) - \underline{\lambda}^0 : (\underline{D}(\underline{q}) \otimes_s \underline{u}(\underline{q}))$$

Basic scheme

Lippmann-Schwinger equation in q-space

$$\underline{\Omega}^{-1}(\underline{q}) \cdot \underline{u}(\underline{q}) = -\underline{\tau}(\underline{q}) \cdot \underline{D}(\underline{q})^*$$

Inverse of the elastic Green tensor

$$\underline{\Omega}^{-1}(\underline{q}) = \underline{D}(\underline{q})^* \cdot \underline{\lambda}^0 \cdot \underline{D}(\underline{q})$$

Reciprocal Lattice (RL) of the grid (●) :

$$\underline{q} = (0, 0, 0), (2\pi, 0, 0) \dots$$

If $\underline{D}(\underline{q}) \neq \underline{0}$ for all $\underline{q} \neq \underline{0}$, then : $\forall \underline{q} \neq \underline{0}, \underline{u}(\underline{q}) = -\underline{\Omega}(\underline{q}) \cdot \underline{\tau}(\underline{q}) \cdot \underline{D}(\underline{q})^*$

here : $D(\underline{q}) = 0$ for $q = (0, \pi), (\pi, 0), (\pi, \pi)$

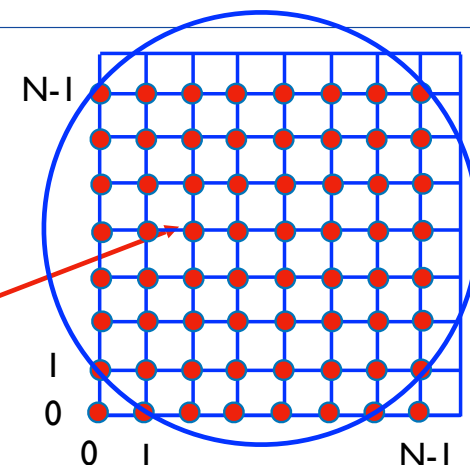
centered scheme is not stable !
oscillations, checkerboarding...

$$\underline{r} : (l, m, n) d$$

$$l = 0, 1, \dots, (N_x - 1)$$

$$\underline{\epsilon}(l, m, n)$$

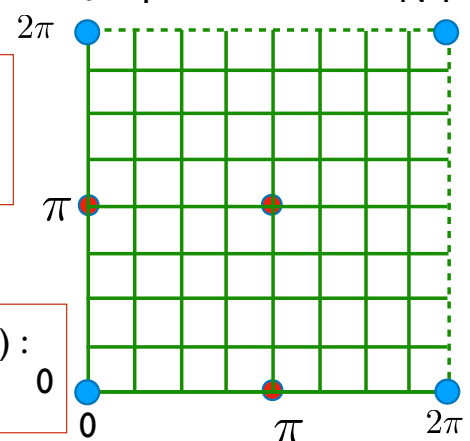
$$\underline{u}(l, m, n)$$



Brillouin zone

$$\underline{q} : \frac{2\pi}{d} \left(\frac{h}{N_x}, \frac{k}{N_y}, \frac{l}{N_z} \right)$$

$$h = 0, 1, \dots, (N_x - 1)$$



The “rotated” staggered Simple Cubic scheme

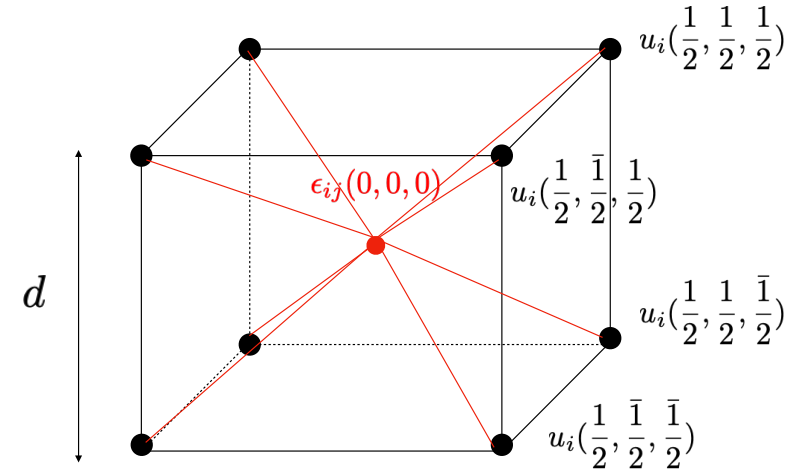
(Saenger et al, 2000;
Willot, 2015)

Discretization :

- cubic grid for the displacements
- cubic grid for the strain (stress, stiffness....)

Stencil :

$$\epsilon_{11}(000) = \frac{1}{4} \left\{ u_1\left(\frac{1}{2} \frac{1}{2} \frac{1}{2}\right) + u_1\left(\frac{1}{2} \bar{1} \frac{1}{2}\right) + u_1\left(\frac{1}{2} \frac{1}{2} \bar{1}\right) + u_1\left(\frac{1}{2} \bar{1} \bar{1}\right) \right. \\ \left. - u_1\left(\frac{1}{2} \frac{1}{2} \frac{1}{2}\right) - u_1\left(\frac{1}{2} \frac{1}{2} \bar{1}\right) - u_1\left(\frac{1}{2} \bar{1} \frac{1}{2}\right) - u_1\left(\frac{1}{2} \bar{1} \bar{1}\right) \right\}$$



Q-space :

$$\underline{\epsilon}(\underline{q}) = \underline{D}(\underline{q}) \otimes_s \underline{u}(\underline{q})$$

DFT of finite difference operators :

$$D_1(q) = \frac{1}{4} (e^{iq_1} - 1) (e^{iq_2} + 1) (e^{iq_3} + 1) \\ D_2(q) = \frac{1}{4} (e^{iq_1} + 1) (e^{iq_2} - 1) (e^{iq_3} + 1) \\ D_3(q) = \frac{1}{4} (e^{iq_1} + 1) (e^{iq_2} + 1) (e^{iq_3} - 1)$$

Equilibrium in q-space :

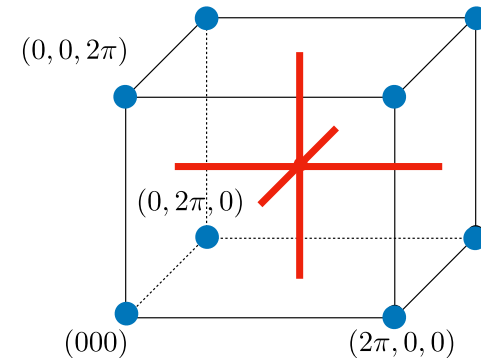
Lippmann–Schwinger
equation

$$\underline{\Omega}^{-1}(\underline{q}) = \underline{D}(\underline{q})^* \cdot \underline{\lambda}^0 \cdot \underline{D}(\underline{q})$$

$$\underline{u}(\underline{q}) = -\underline{\Omega}(\underline{q}) \cdot \underline{\tau}(\underline{q}) \cdot \underline{D}(\underline{q})^*$$

$$D_i(q) = 0 \quad \text{for :} \quad \begin{aligned} q &= (\pi, \pi, q_z) & \forall q_z \\ q &= (\pi, q_y, \pi) & \forall q_y \\ q &= (q_x, \pi, \pi) & \forall q_x \end{aligned}$$

Reciprocal Lattice (RL)
of the simple cubic grids



→ Solver is unstable : stress oscillations, overshoot...

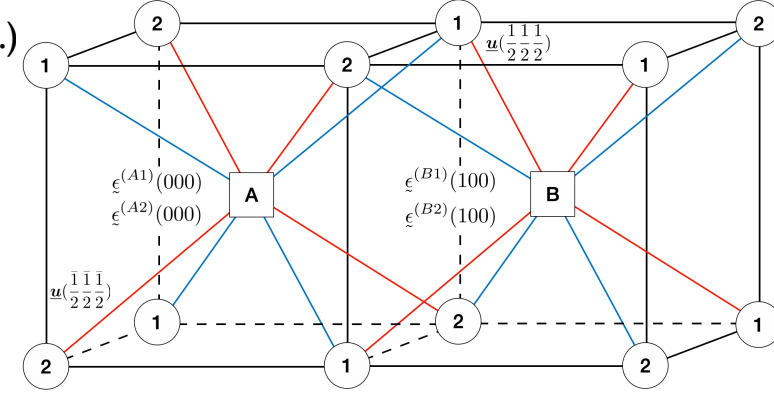
A tetrahedral stencil on a Simple Cubic grid (I) Finel, CMAME (2025)

Discretization : cubic grids for the displacements and for the strain (stress, stiffness....)

Stencil : subdivide the displacement grid into 2 FCC lattices ! $\longrightarrow$ 2 stencils :

$$\epsilon_{11}^{(A1)}(000) = \frac{1}{2} \left\{ u_1^{(1)} \left(\frac{1}{2} \frac{1}{2} \frac{1}{2} \right) + u_1^{(1)} \left(\frac{1}{2} \frac{\bar{1}}{2} \frac{\bar{1}}{2} \right) - u_1^{(1)} \left(\frac{\bar{1}}{2} \frac{\bar{1}}{2} \frac{1}{2} \right) - u_1^{(1)} \left(\frac{\bar{1}}{2} \frac{1}{2} \frac{\bar{1}}{2} \right) \right\} \quad \epsilon_{11}^{(B1)}(000) = \dots$$

$$\epsilon_{11}^{(A2)}(000) = \frac{1}{2} \left\{ u_1^{(2)} \left(\frac{1}{2} \frac{\bar{1}}{2} \frac{1}{2} \right) + u_1^{(2)} \left(\frac{1}{2} \frac{1}{2} \frac{\bar{1}}{2} \right) - u_1^{(2)} \left(\frac{\bar{1}}{2} \frac{1}{2} \frac{1}{2} \right) - u_1^{(2)} \left(\frac{\bar{1}}{2} \frac{\bar{1}}{2} \frac{\bar{1}}{2} \right) \right\} \quad \epsilon_{11}^{(B2)}(000) = \dots$$



Q-space : Fourier transforms on the FCC sublattices :

$$\underline{u}^{(1)}(\underline{q}) = \frac{1}{N} \sum_{\underline{r} \in \textcircled{1}} \underline{u}(\underline{r}) \exp(-i\underline{q} \cdot \underline{r}) \quad \underline{u}^{(2)}(\underline{q}) = \frac{1}{N} \sum_{\underline{r} \in \textcircled{2}} \underline{u}(\underline{r}) \exp(-i\underline{q} \cdot \underline{r})$$

$\longrightarrow$ 2 Lippmann-Schwinger equations with the same Green function :

$$\forall \underline{q} \neq (000)^*, \quad \underline{\Omega}(\underline{q})^{-1} \cdot \underline{u}^{(1)}(\underline{q}) = -\{ \tau^{(A1)}(\underline{q}) \cdot \overline{\underline{D}(\underline{q})} - \tau^{(B1)}(\underline{q}) \cdot \underline{D}(\underline{q}) \}$$

$$\forall \underline{q} \neq (000)^*, \quad \underline{\Omega}(\underline{q})^{-1} \cdot \underline{u}^{(2)}(\underline{q}) = -\{ \tau^{(B2)}(\underline{q}) \cdot \overline{\underline{D}(\underline{q})} - \tau^{(A2)}(\underline{q}) \cdot \underline{D}(\underline{q}) \}$$

$$\underline{\Omega}(\underline{q})^{-1} = \overline{\underline{D}(\underline{q})} \cdot \underline{\lambda}^0 \cdot \underline{D}(\underline{q}) + \underline{D}(\underline{q}) \cdot \underline{\lambda}^0 \cdot \overline{\underline{D}(\underline{q})}.$$

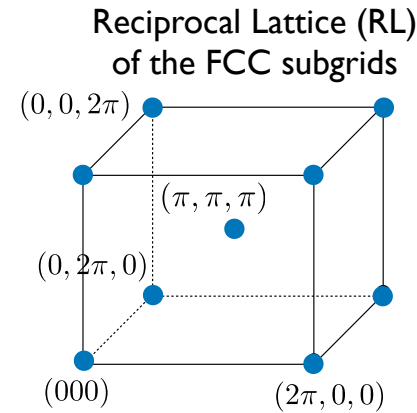
$$D_1(\underline{q}) = \frac{1}{2} \left\{ \exp\left(\frac{i}{2}(q_1 + q_2 + q_3)\right) + \exp\left(\frac{i}{2}(q_1 - q_2 - q_3)\right) - \exp\left(\frac{i}{2}(-q_1 + q_2 - q_3)\right) - \exp\left(\frac{i}{2}(-q_1 - q_2 + q_3)\right) \right\}$$

$$D_2(\underline{q}) = \frac{1}{2} \left\{ \exp\left(\frac{i}{2}(q_1 + q_2 + q_3)\right) - \exp\left(\frac{i}{2}(q_1 - q_2 - q_3)\right) + \exp\left(\frac{i}{2}(-q_1 + q_2 - q_3)\right) - \exp\left(\frac{i}{2}(-q_1 - q_2 + q_3)\right) \right\}$$

$$D_3(\underline{q}) = \frac{1}{2} \left\{ \exp\left(\frac{i}{2}(q_1 + q_2 + q_3)\right) - \exp\left(\frac{i}{2}(q_1 - q_2 - q_3)\right) - \exp\left(\frac{i}{2}(-q_1 + q_2 - q_3)\right) + \exp\left(\frac{i}{2}(-q_1 - q_2 + q_3)\right) \right\}$$

$$\underline{D}(\underline{q}) = \underline{0} \text{ for } \underline{q} = \underline{0}$$

$$\text{and } \underline{q} = (\pi, \pi, \pi) !!!$$



$\underline{D}(\underline{q}) \neq \underline{0}$ for all $\underline{q} \notin \text{RL}$: **Solver is stable !**

$$\forall \underline{q} \neq (000)^*, \quad \underline{u}^{(1)}(\underline{q}) = -\underline{\Omega}(\underline{q}) \cdot \{ \tau^{(A1)}(\underline{q}) \cdot \overline{\underline{D}(\underline{q})} - \tau^{(B1)}(\underline{q}) \cdot \underline{D}(\underline{q}) \}$$

$$\forall \underline{q} \neq (000)^*, \quad \underline{u}^{(2)}(\underline{q}) = -\underline{\Omega}(\underline{q}) \cdot \{ \tau^{(B2)}(\underline{q}) \cdot \overline{\underline{D}(\underline{q})} - \tau^{(A2)}(\underline{q}) \cdot \underline{D}(\underline{q}) \}$$

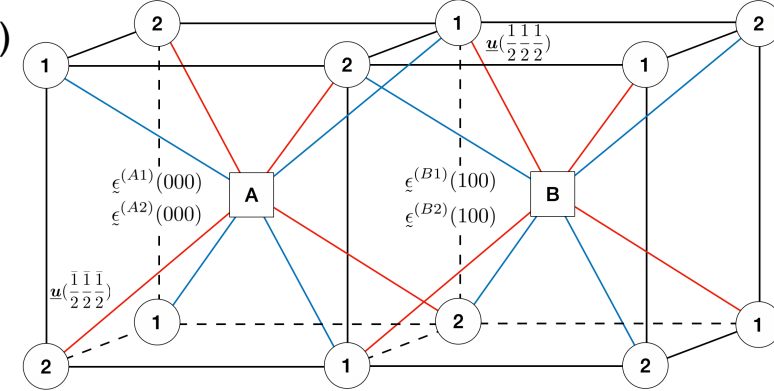
A tetrahedral stencil on a Simple Cubic grid (2) Finel, CMAME (2025)

Discretization : cubic grid for the displacements and for the strain (stress, stiffness....)

Stencil : subdivide the displacement grid into 2 FCC lattices ! $\longrightarrow$ 2 stencils :

$$\epsilon_{11}^{(A1)}(000) = \frac{1}{2} \left\{ u_1^{(1)}\left(\frac{1}{2} \frac{1}{2} \frac{1}{2}\right) + u_1^{(1)}\left(\frac{1}{2} \frac{\bar{1}}{2} \frac{\bar{1}}{2}\right) - u_1^{(1)}\left(\frac{\bar{1}}{2} \frac{\bar{1}}{2} \frac{1}{2}\right) - u_1^{(1)}\left(\frac{\bar{1}}{2} \frac{1}{2} \frac{\bar{1}}{2}\right) \right\} \quad \epsilon_{11}^{(B1)}(000) = \dots$$

$$\epsilon_{11}^{(A2)}(000) = \frac{1}{2} \left\{ u_1^{(2)}\left(\frac{1}{2} \frac{\bar{1}}{2} \frac{1}{2}\right) + u_1^{(2)}\left(\frac{1}{2} \frac{1}{2} \frac{\bar{1}}{2}\right) - u_1^{(2)}\left(\frac{\bar{1}}{2} \frac{1}{2} \frac{1}{2}\right) - u_1^{(2)}\left(\frac{\bar{1}}{2} \frac{\bar{1}}{2} \frac{\bar{1}}{2}\right) \right\} \quad \epsilon_{11}^{(B2)}(000) = \dots$$



Q-space : Fourier transforms on the FCC sublattices :

$$\underline{u}^{(1)}(\underline{q}) = \frac{1}{N} \sum_{\underline{r} \in \textcircled{1}} \underline{u}(\underline{r}) \exp(-i\underline{q} \cdot \underline{r}) \quad \underline{u}^{(2)}(\underline{q}) = \frac{1}{N} \sum_{\underline{r} \in \textcircled{2}} \underline{u}(\underline{r}) \exp(-i\underline{q} \cdot \underline{r})$$

$\longrightarrow$ 2 Lippmann-Schwinger equations with the same Green function :

$$\begin{aligned} \forall \underline{q} \neq (000)^*, \quad \underline{\Omega}(\underline{q})^{-1} \cdot \underline{u}^{(1)}(\underline{q}) &= -\{\tau^{(A1)}(\underline{q}) \cdot \overline{\underline{D}(\underline{q})} - \tau^{(B1)}(\underline{q}) \cdot \underline{D}(\underline{q})\} \\ \forall \underline{q} \neq (000)^*, \quad \underline{\Omega}(\underline{q})^{-1} \cdot \underline{u}^{(2)}(\underline{q}) &= -\{\tau^{(B2)}(\underline{q}) \cdot \overline{\underline{D}(\underline{q})} - \tau^{(A2)}(\underline{q}) \cdot \underline{D}(\underline{q})\} \end{aligned}$$

$$\underline{\Omega}(\underline{q})^{-1} = \overline{\underline{D}(\underline{q})} \cdot \underline{\lambda}^0 \cdot \underline{D}(\underline{q}) + \underline{D}(\underline{q}) \cdot \underline{\lambda}^0 \cdot \overline{\underline{D}(\underline{q})}.$$

that we can collapse :

$$\underline{u}(\underline{q}) = \underline{u}^{(1)}(\underline{q}) + \underline{u}^{(2)}(\underline{q})$$

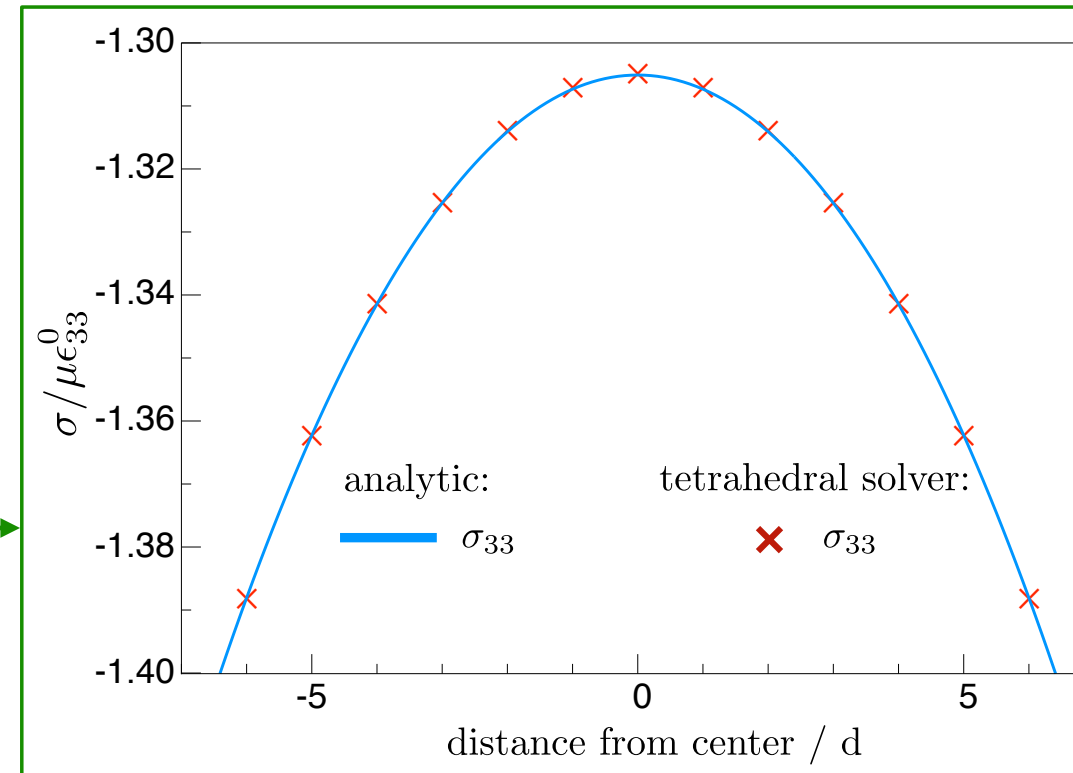
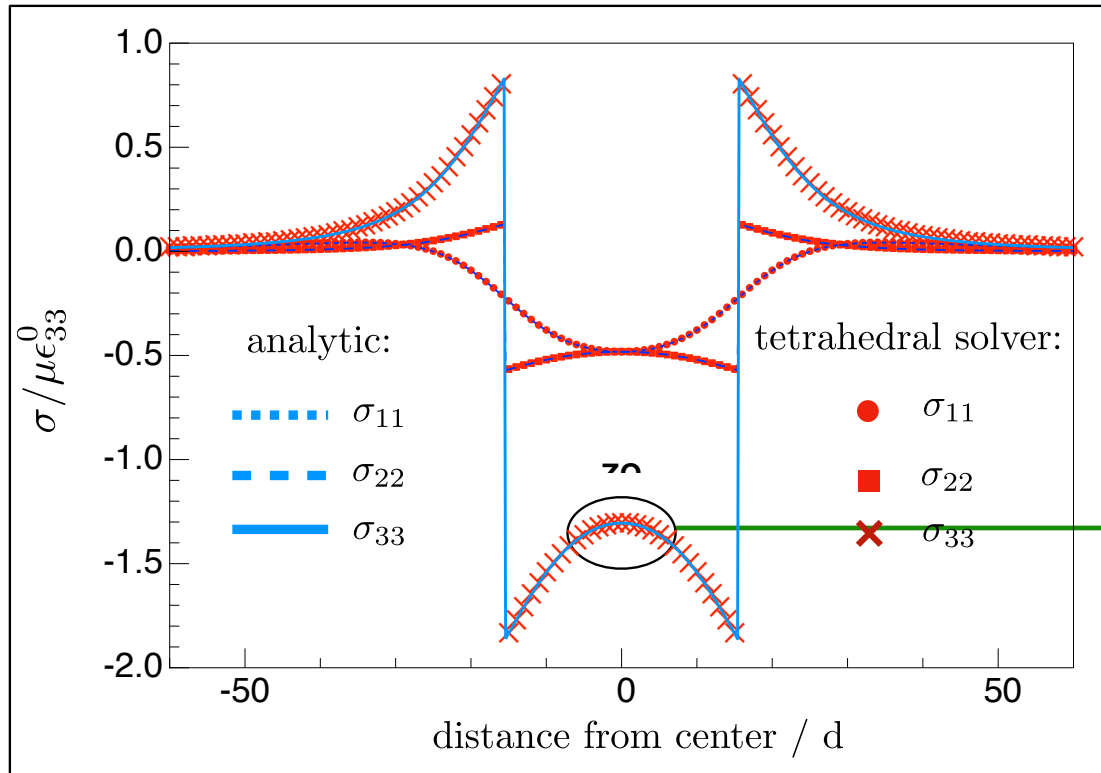
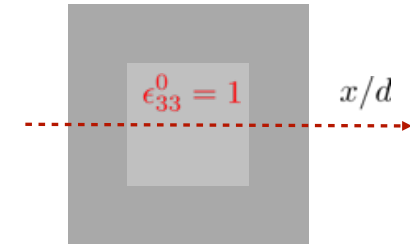
$$\begin{aligned} \tau^{(T1)}(\underline{q}) &= \tau^{(A1)}(\underline{q}) + \tau^{(B2)}(\underline{q}) \\ \tau^{(T2)}(\underline{q}) &= \tau^{(A2)}(\underline{q}) + \tau^{(B1)}(\underline{q}) \end{aligned}$$

$$\forall \underline{q} \neq (000)^*, \quad \underline{u}(\underline{q}) = -\underline{\Omega}(\underline{q}) \cdot \{\tau^{(T1)}(\underline{q}) \cdot \overline{\underline{D}(\underline{q})} - \tau^{(T2)}(\underline{q}) \cdot \underline{D}(\underline{q})\},$$

Quality of the tetrahedral solver (I)

Cubic inclusion with eigenstrain :

- 3D simple cubic grid 256x256x256
- cubic precipitate of size 32x32x32 with eigenstrain $\epsilon_{33}^0 = 1$
- homogeneous isotropic elasticity : $\mu = 132.30$ GPa $\nu = 0.26$



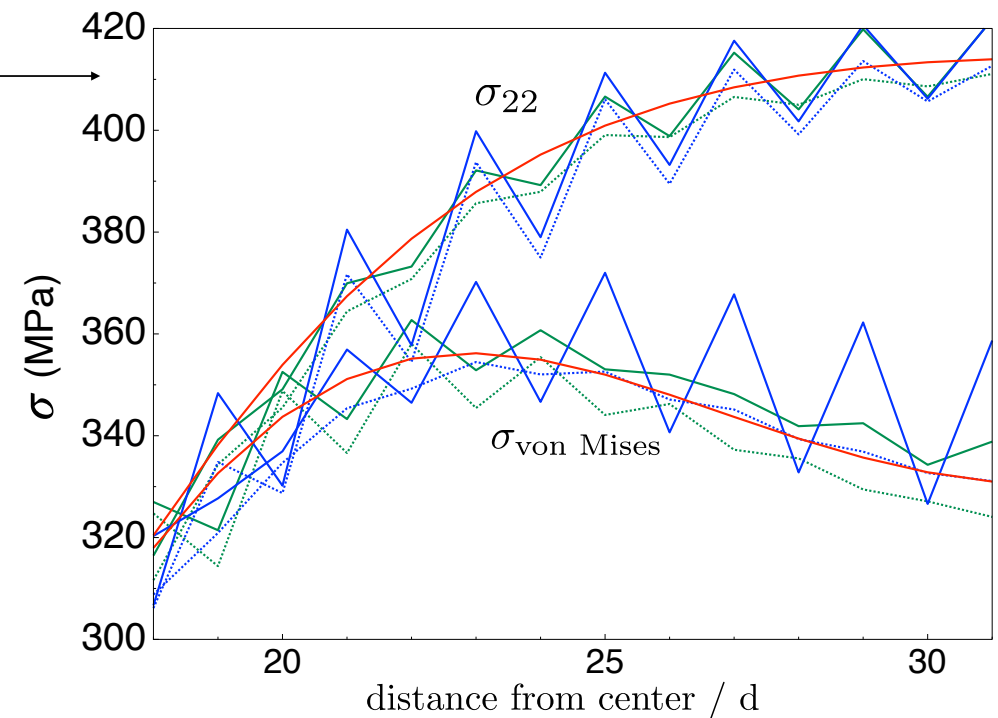
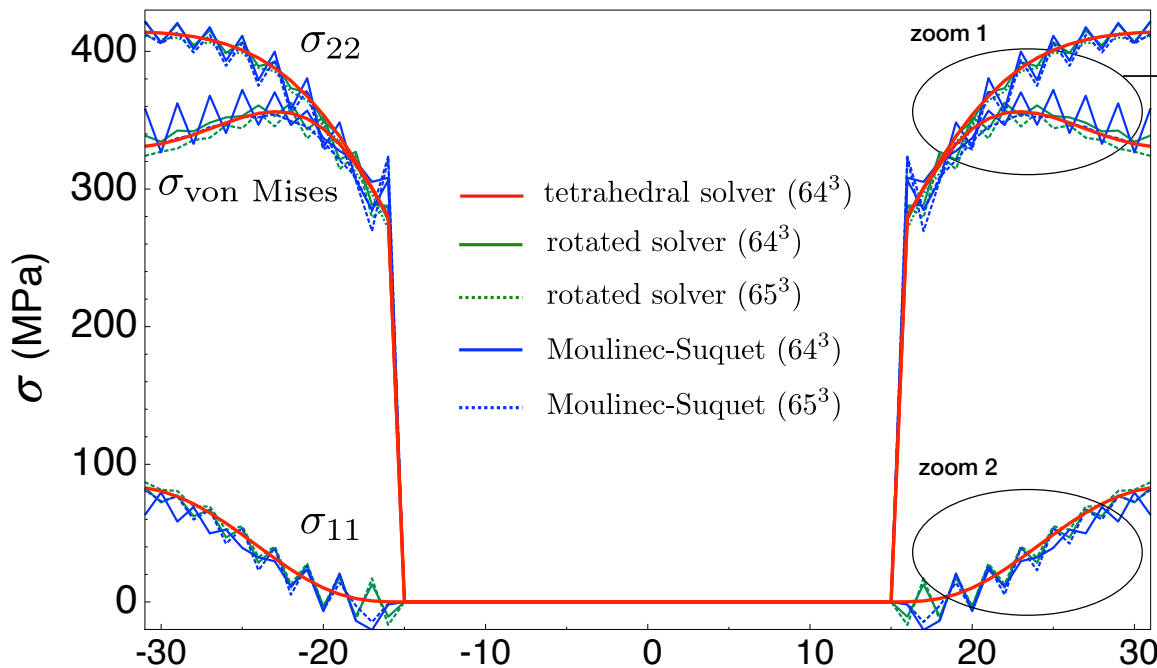
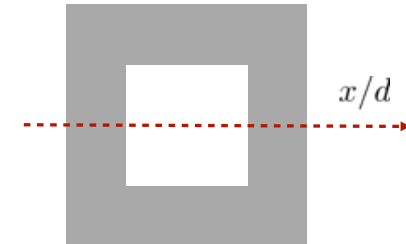
Quality of the tetrahedral solver (2)



Cubic void :

- 3D simple cubic grid $64 \times 64 \times 64$
- cubic cavity ($l = 32 d$)
- hydrostatic pressure (300 MPa)
- isotropic elasticity : $\mu = 132.30 \text{ GPa}$ $\nu = 0.26$

- tetrahedral solver
- rotated solver
- Moulinec-Suquet solver



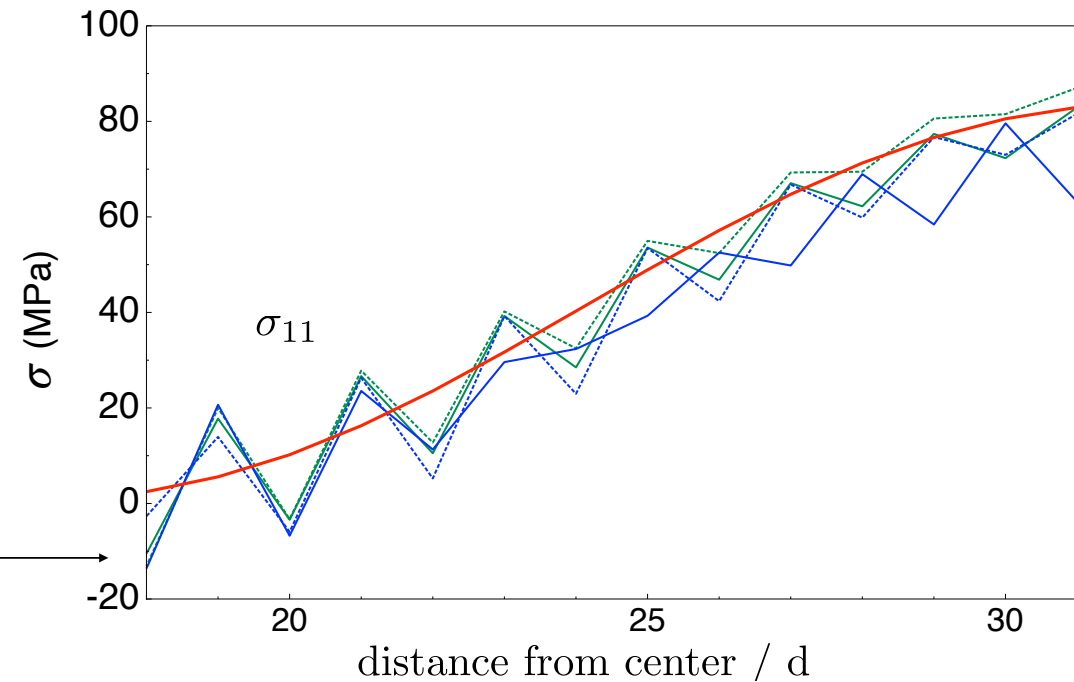
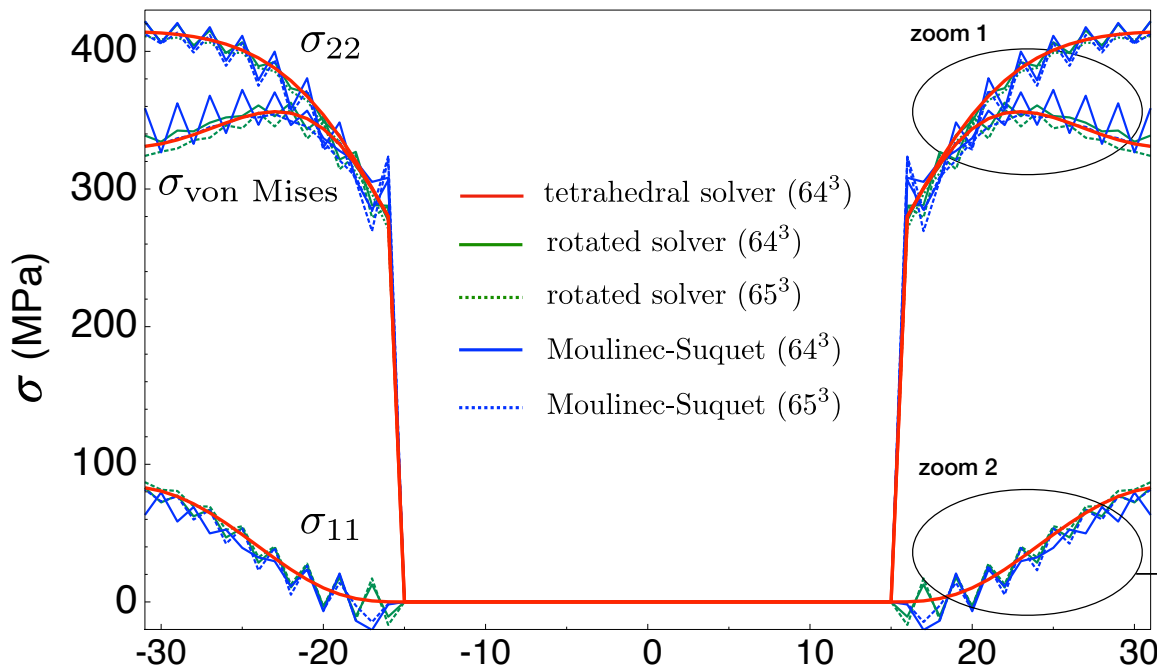
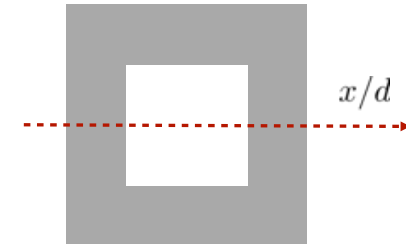
Quality of the tetrahedral solver (2)



Cubic void :

- 3D simple cubic grid $64 \times 64 \times 64$
- cubic cavity ($l = 32 d$)
- hydrostatic pressure (300 MPa)
- isotropic elasticity : $\mu = 132.30 \text{ GPa}$ $\nu = 0.26$

- tetrahedral solver
- rotated solver
- Moulinec-Suquet solver

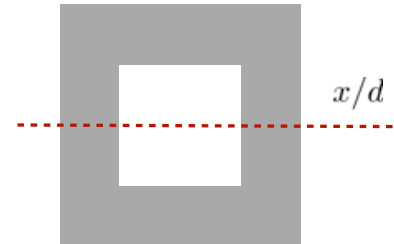


Quality of the tetrahedral solver (2)

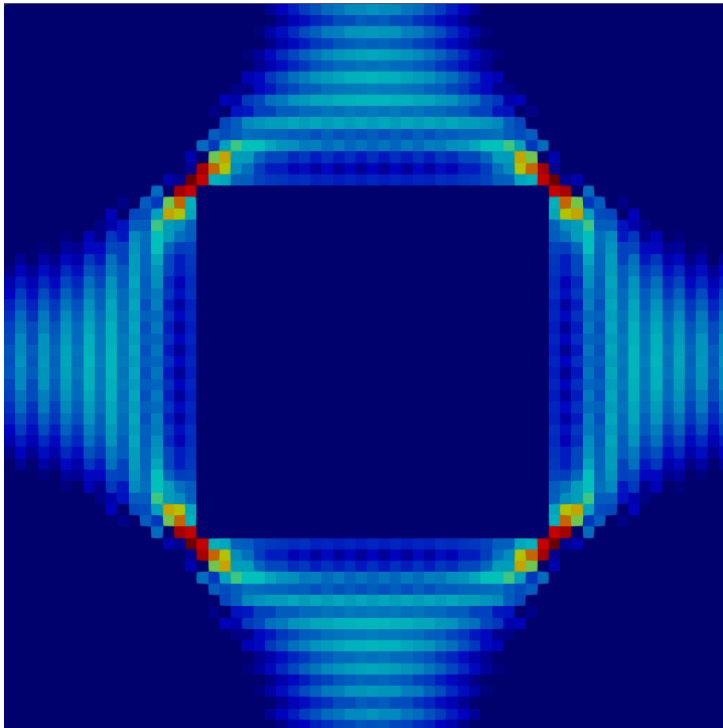
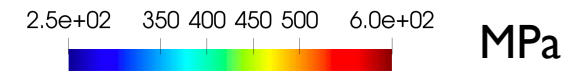


Cubic void :

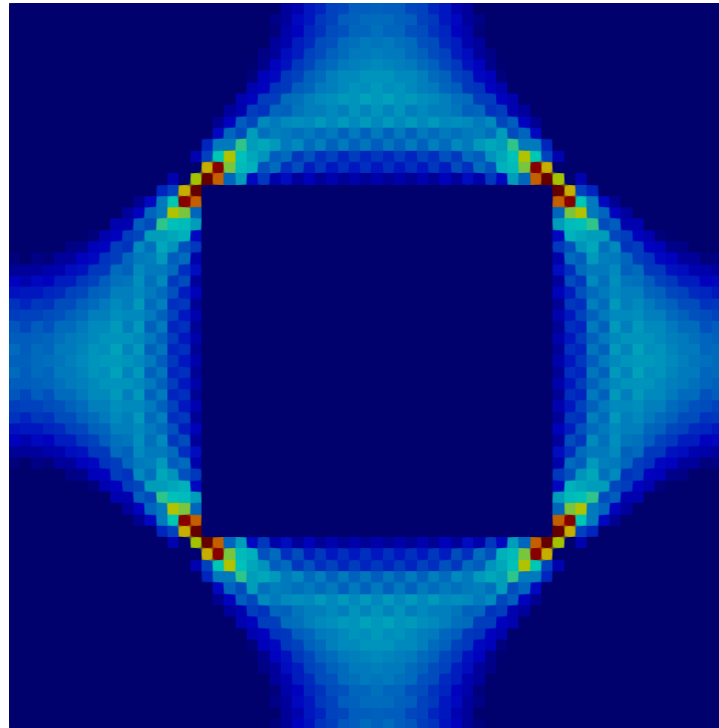
- 3D simple cubic grid 64x64x64
- cubic cavity ($l = 32 d$)
- hydrostatic pressure (300 MPa)
- isotropic elasticity : $\mu = 132.30$ GPa $\nu = 0.26$



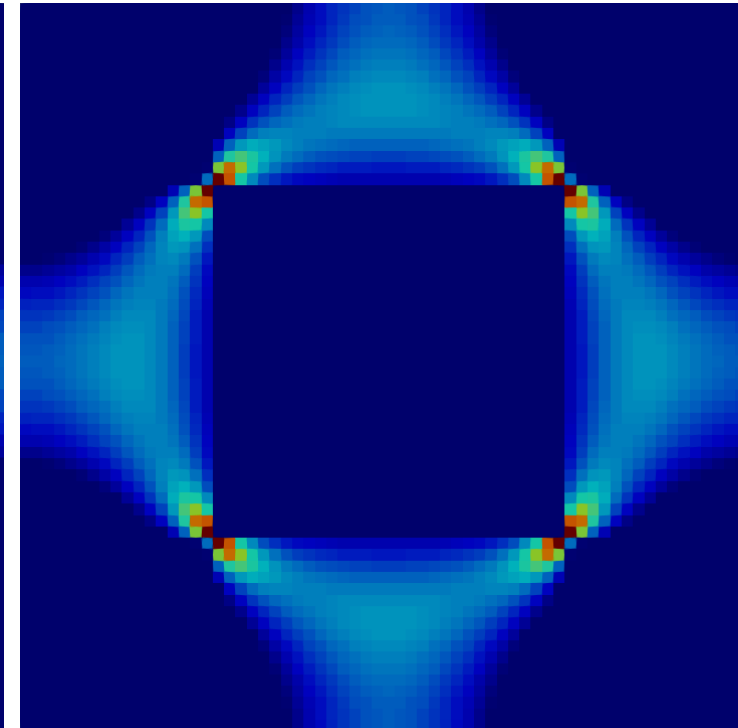
von Mises stress



Moulinec-Suquet's scheme



Rotated scheme

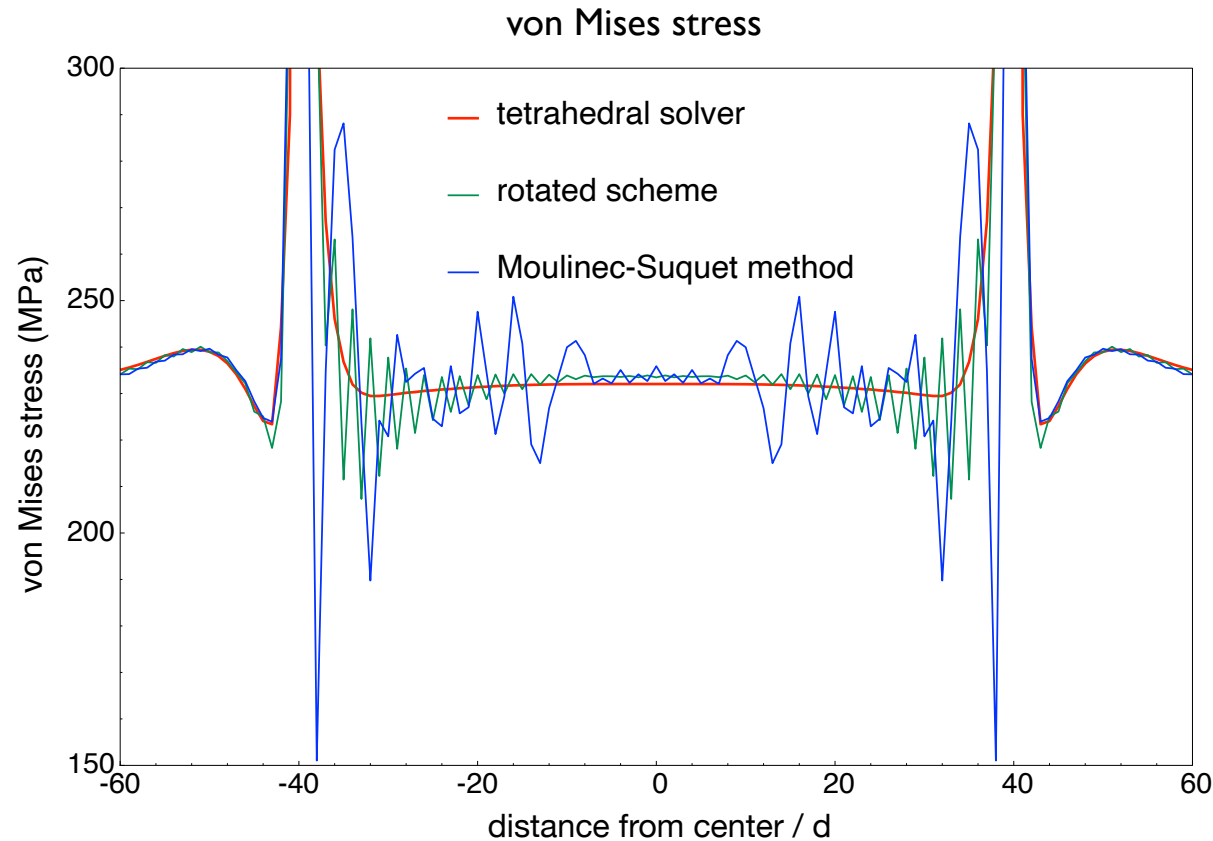
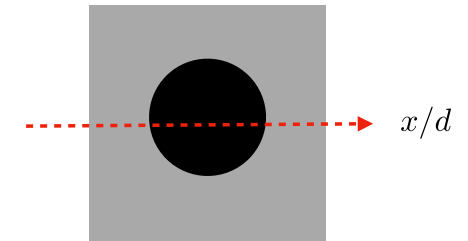


Tetrahedral solver

Quality of the tetrahedral solver (3)

Hard spherical inclusion in a soft matrix :

- polyamide matrix : $E = 2.1 GPa$ $\nu = 0.3$
- spherical glass inclusion : $E = 72 GPa$ $\nu = 0.22$
- applied strain : $\epsilon_{11}^a = 0.05$
- 3D simple cubic grid $128 \times 128 \times 128$
- spherical inclusion $R = 40 d$

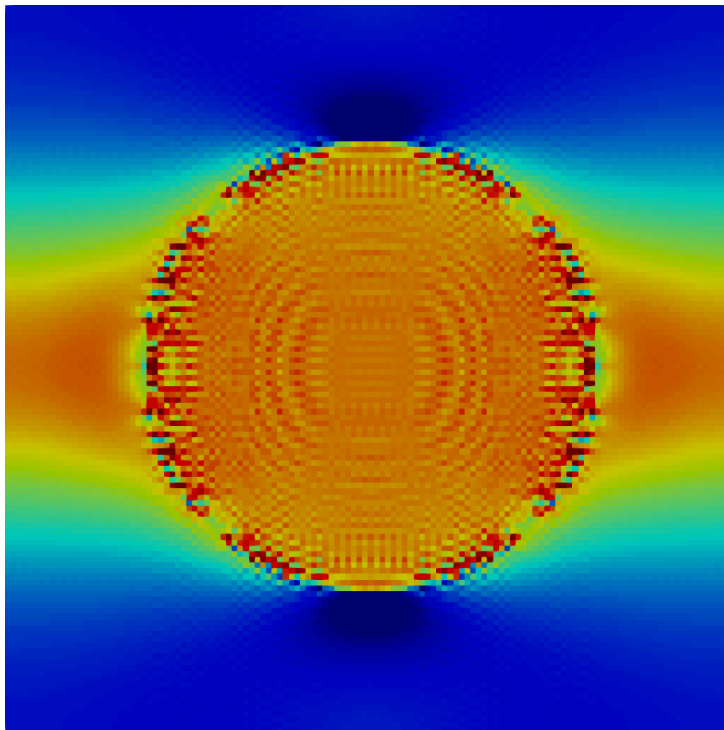


Quality of the tetrahedral solver (3)

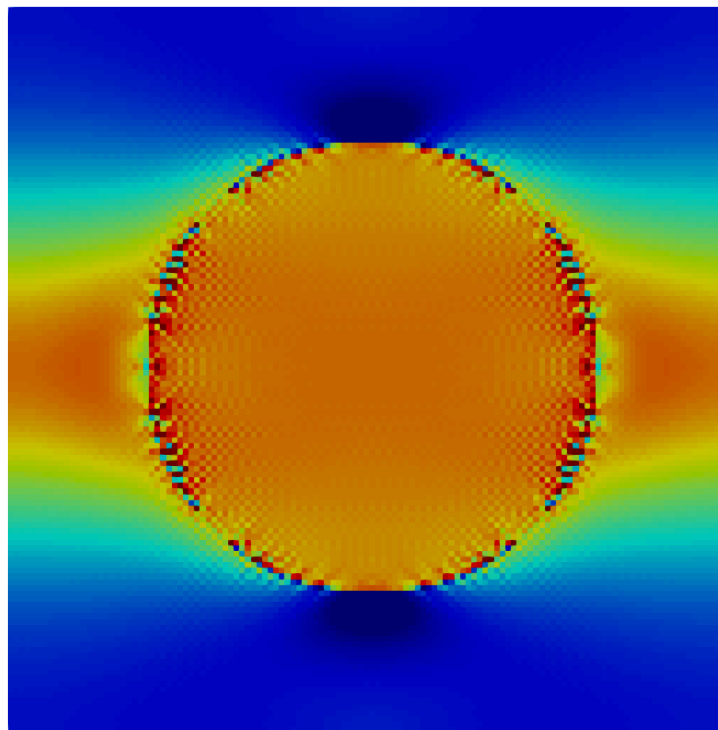
Hard spherical inclusion in a soft matrix :

- polyamide matrix : $E = 2.1GPa$ $\nu = 0.3$
- spherical glass inclusion : $E = 72GPa$ $\nu = 0.22$
- applied strain : $\epsilon_{11}^a = 0.05$
- 3D simple cubic grid $128 \times 128 \times 128$
- spherical inclusion $R = 40 d$

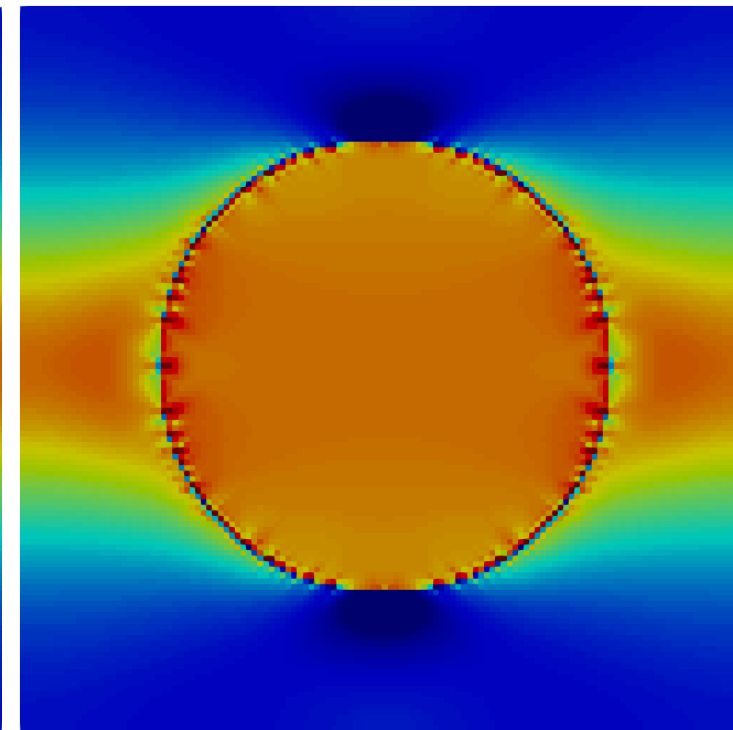
von Mises stress



Moulinec-Suquet's scheme



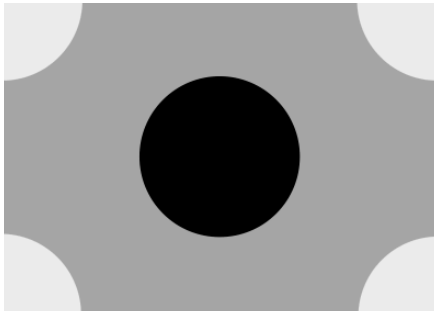
Rotated scheme



Tetrahedral solver

Quality of the tetrahedral solver (4)

 Microstructure with a “double contrast” :



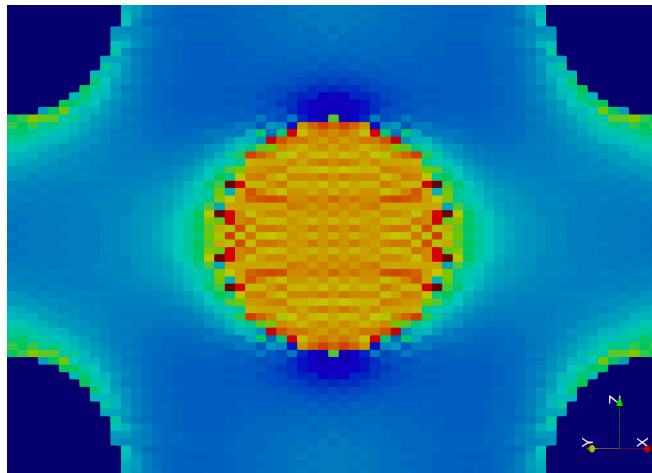
	matrix	soft incl.	hard incl.
Shear modulus	G	$10^{-5} G$	$10^5 G$
Poisson ratio	0.3	0.3	0.3

- 3D simple cubic grid $64 \times 64 \times 64$
- spherical inclusions $R = 16 d$

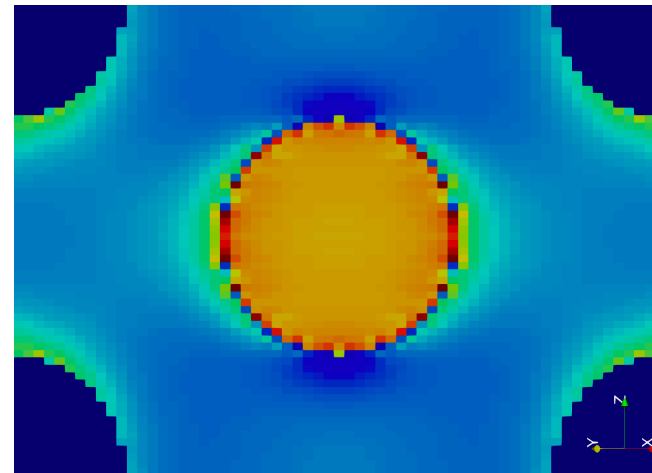
→ “Basic scheme” does not converge ($N = 10^4$ iterations not enough to reach $\epsilon_{L^2} = 10^{-10}$)

→ adaptation of the polarization scheme (Monchiet-Bonnet, 2012) to the tetrahedral stencil

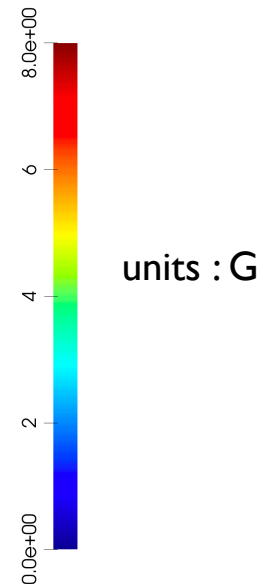
von Mises stress



Rotated scheme

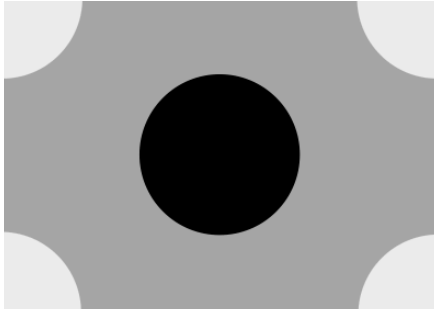


Tetrahedral solver



Quality of the tetrahedral solver (4)

Microstructure with a “double contrast” :



	matrix	soft incl.	hard incl.
Shear modulus	G	$10^{-5} G$	$10^5 G$
Poisson ratio	0.3	0.3	0.3

- 3D simple cubic grid 64x64x64
- spherical inclusions $R = 16 d$

- “Basic scheme” does not converge ($N = 10^4$ iterations not enough to reach $\epsilon_{L^2} = 10^{-10}$)
- adaptation of the polarization scheme (Monchiet-Bonnet, 2012) to the tetrahedral stencil

Rate of convergence vs contrast :

Table 1

3D medium with double contrast : convergence rate of the polarization-based algorithm associated with the tetrahedral stencil (Algorithm 3 with $\gamma = 0$); number of iterates as a function of the double contrast χ to reach equilibrium with the precision $\epsilon_{pol} = 10^{-10}$.

χ	10	10^2	10^3	10^4	10^5	10^6
Iterates	67	237	339	386	425	462

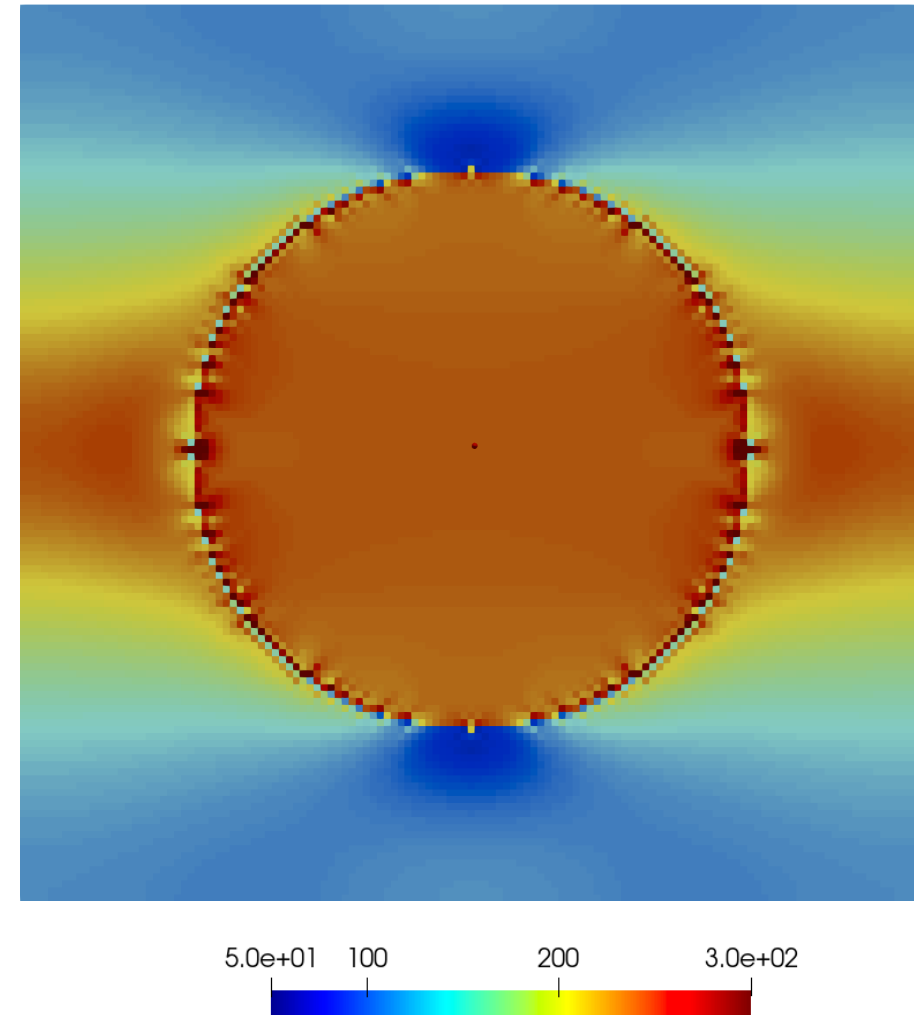
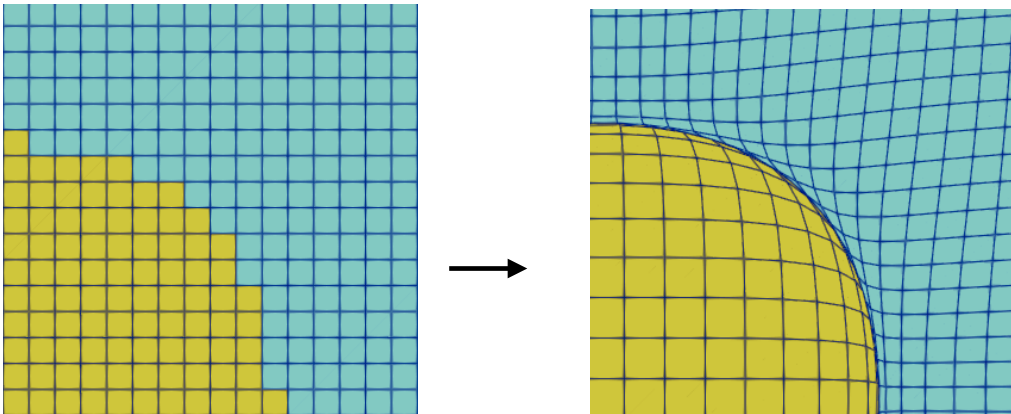
- convergence is linear

-

Problem of “vocalisation”

- FFT algorithms need regular grids
- inaccurate discretization of “non-conform” interfaces
- steps / corners generate artificial high stress concentrations...

Use of “deformed” grids...



Outline

1. The Sharp Phase Field Method (S-PFM)
2. A robust FFT-based solver for microstructures with sharp interfaces
3. FFT-solvers on non-uniform grids (in progress...)

Conclusion

1. The Sharp Phase Field Method :

- a phase field method that permits interface to be resolved with, typically, only 1 grid point....

2. A tetrahedron-based FFT solver :

- mathematically stable, for any elastic contrast
- fast convergence (even in presence of voids...)

3. FFT solvers and non-uniform grids

- “remapping” : proposition of a simple (and fast) methodology
- mechanical problem in computational space : “virtual” material with very strong elastic contrasts (elastic tensor, eigenstrain)
- need for a “robust” FFT solver (discretisation stencil and resolution of equilibrium)