
## 3ième partie :

# Sharp Phase Field Method

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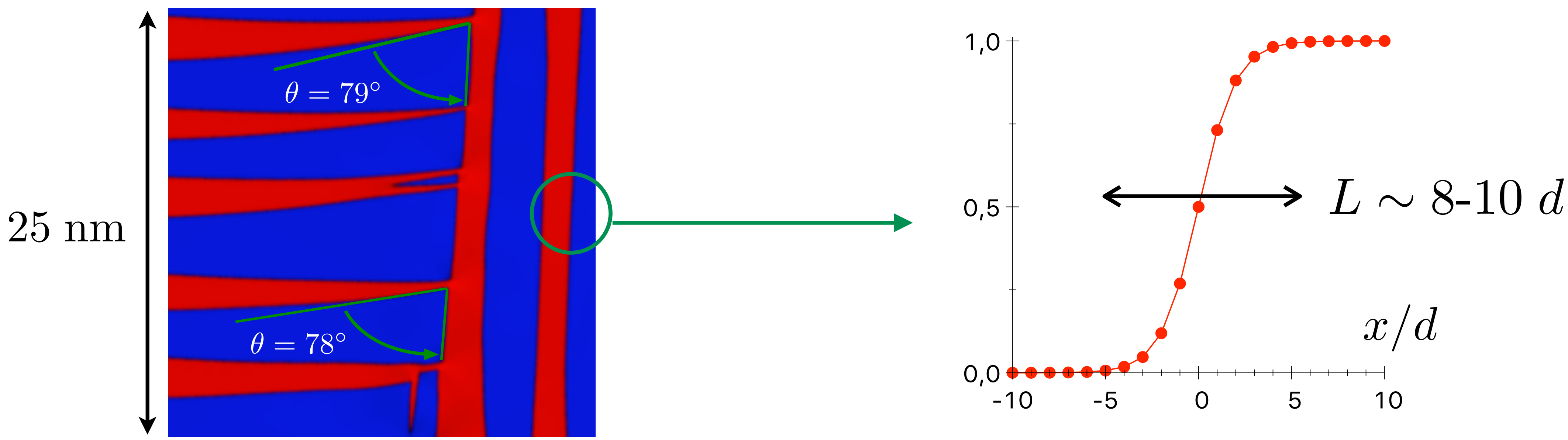
# “Classical” Phase Field Method

## Continuous formulation ⟶ diffuses interfaces !!! :




- Numerics : discrete grid, grid spacing *d*
- No pinning : *d* << *L* ⟶ limitation on accessible linear dimension
- 3D simulations computationally intensive

## What we want :

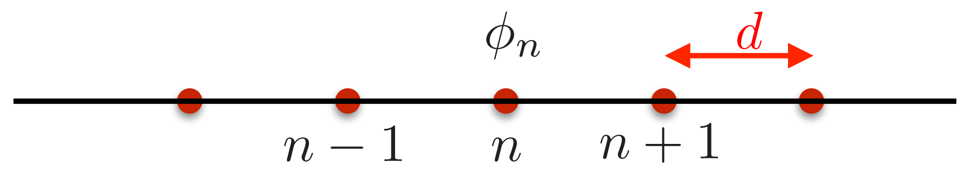
- A phase field method with sharp interfaces on a grid with a finite grid spacing
- with no pinning on the grid, even if the interface thickness $l$ and grid spacing $d$ are such that : $l \ll d$
- Ideally : interface width reduced to only one grid point !

# The Sharp Phase Field pour Method (S-PFM)

## A discrete formulation !

*Finel et al, PRL (2018)*

Consider a 1D lattice :




Discrete free energy functional :

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

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

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

$\longrightarrow$ Question :

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

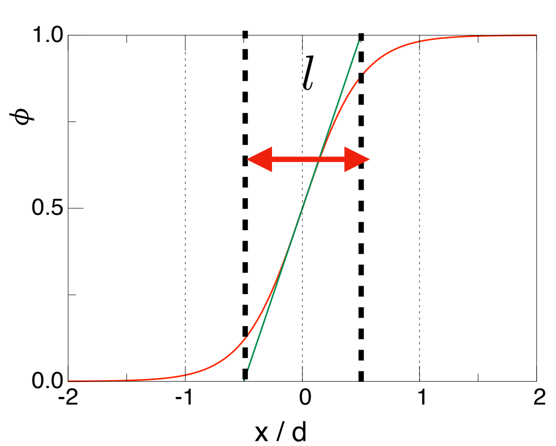
$\longrightarrow$ Procedure :

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

- i.e. look for a function $f(x)$ such that, if $\phi_n = f(n\,d - x_0)$, Eq. 1 becomes an ODE independent of $x_0$ !!!

$\longrightarrow$ Choice :

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




Then : $2\phi_{n\pm1} - 1 = \dfrac{(2\phi_n - 1) \pm \alpha}{1 \pm (2\phi_n - 1)\alpha}$

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

Eq. 1 :

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

Solution :

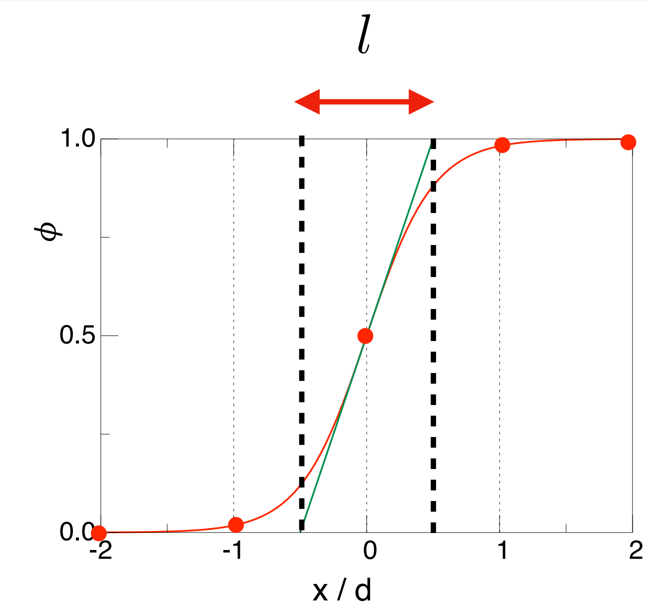
$$g(\phi) = \frac{\lambda}{4\,d^2}\{\frac{\alpha^2 - 1}{\alpha^2}\log[1 - \alpha^2(1-2\phi)^2] - (1-2\phi)^2\}$$

# The Sharp Phase Field pour Method (S-PFM)

## *Landau potential*

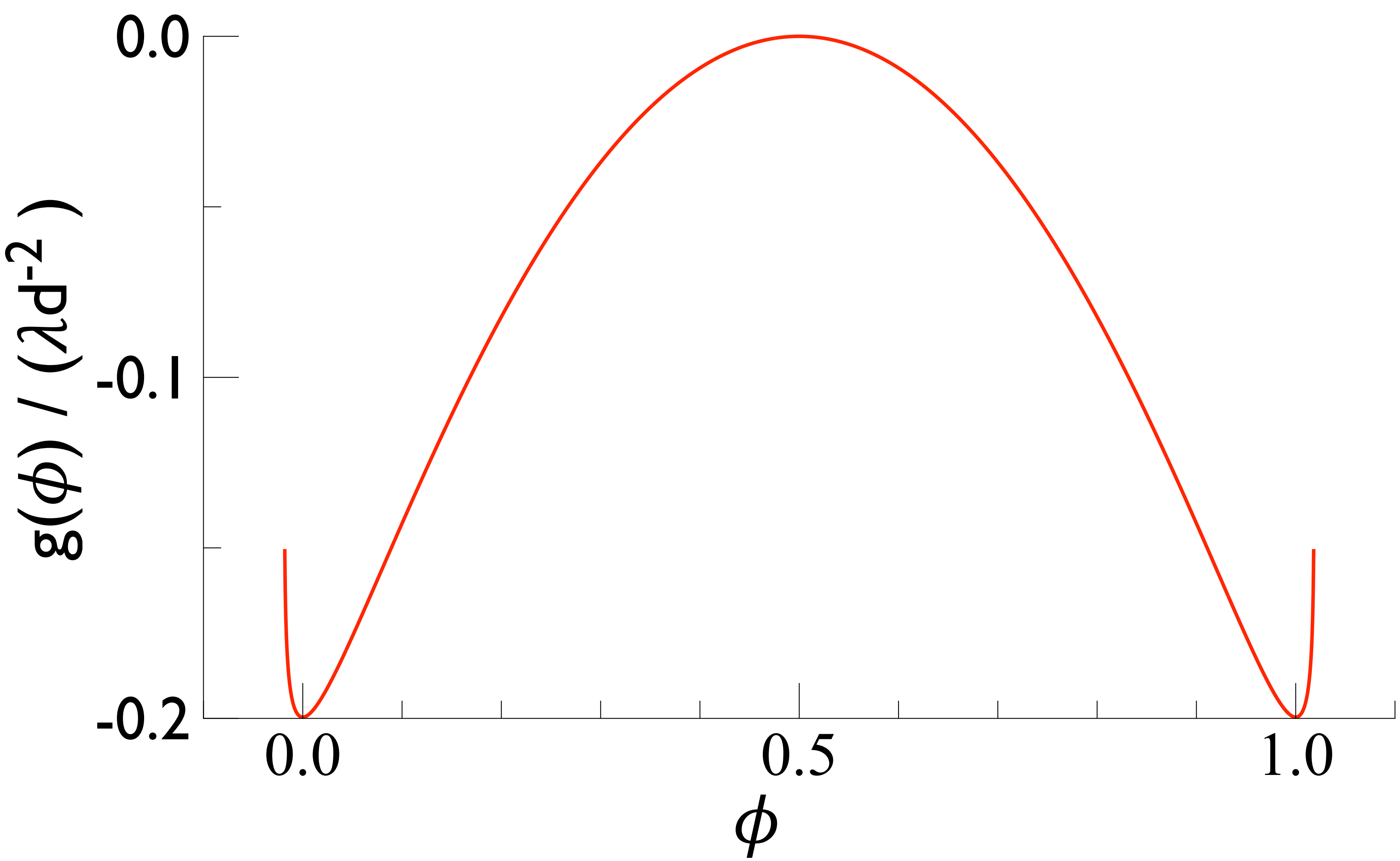
$$g(\phi) = \frac{\lambda}{4\,d^2}\,\{\frac{\alpha^2-1}{\alpha^2}\log[1-\alpha^2(1-2\phi)^2]\;-\;(1-2\phi)^2\}$$

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



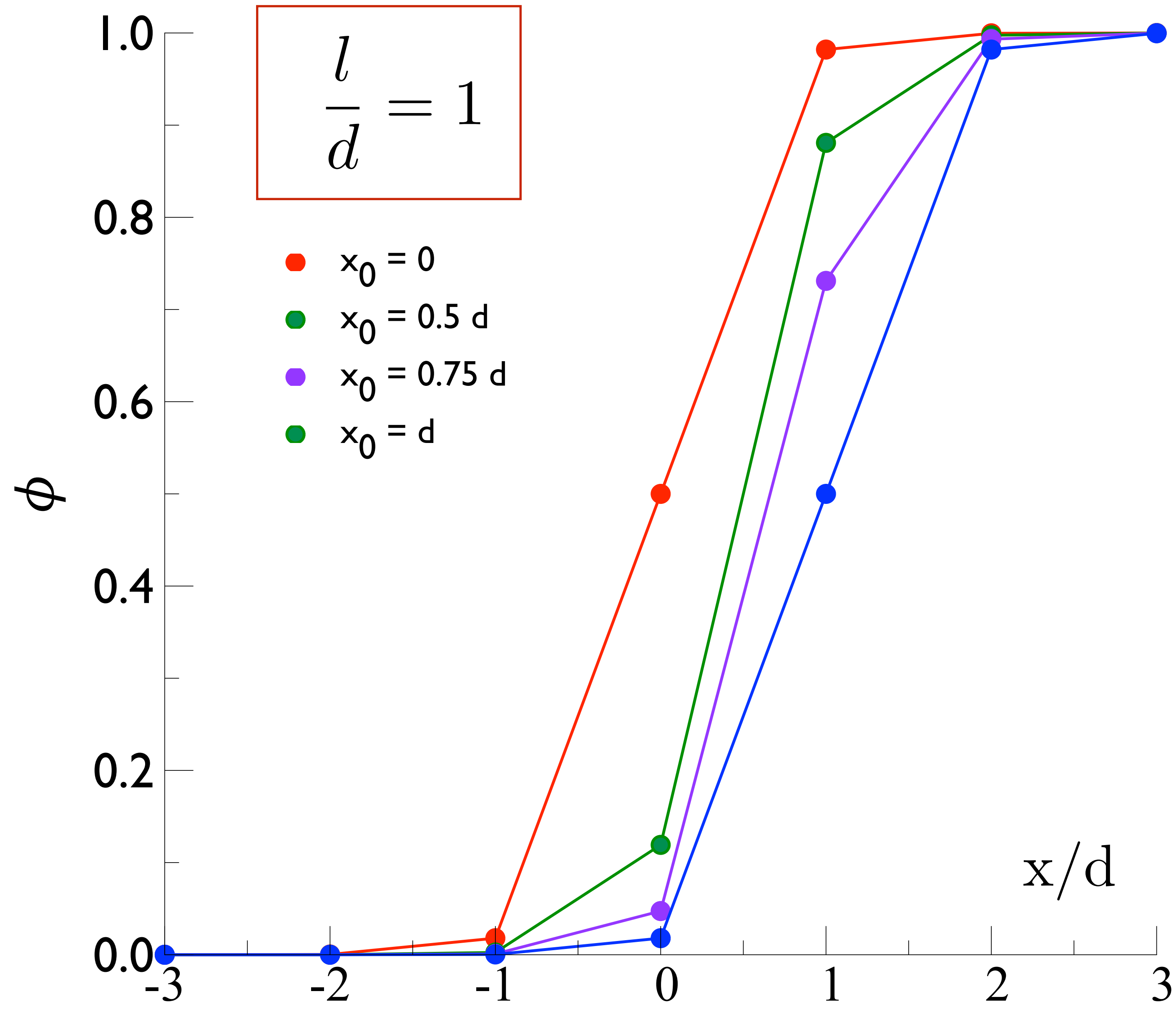

⟶ Exemple :

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



# The Sharp Phase Field pour Method (S-PFM)

*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

## 2D - 3D :

- no solution $g(\phi)$ such that $\sigma_{int}$ is *exactly* invariant by translation along all directions
- no way to recover exact translational and rotational invariances on a discrete lattice

$\longrightarrow$ we proceed as follows :

- select a plane family $(h_1k_1l_1)$ along which we impose continuous translational invariance
- to recover rotational invariance, select $(n-1)$ other families $(h_2k_2l_2)$ ... $(h_nk_nl_n)$ and impose :

$$\sigma(h_1k_1l_1) = \sigma(h_2k_2l_2) = \ldots = \sigma(h_nk_nl_n) \quad \text{Eq. I}$$

- need $(n-1)$ degrees of freedom
- extend gradient terms to $n^{th}$ neighbours, with weighting coefficients $\gamma_i$ !

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

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

$$d_i = ||\vec{r}_i(.)|| \qquad \nu_i = \frac{3}{m_i}$$

- look for a $g(\phi)$ and weighting coefficients $\{\gamma_1, \ldots, \gamma_{n-1}\}$ to fulfil Eq. I and translational invariance along $(h_1k_1l_1)$
- solution :

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

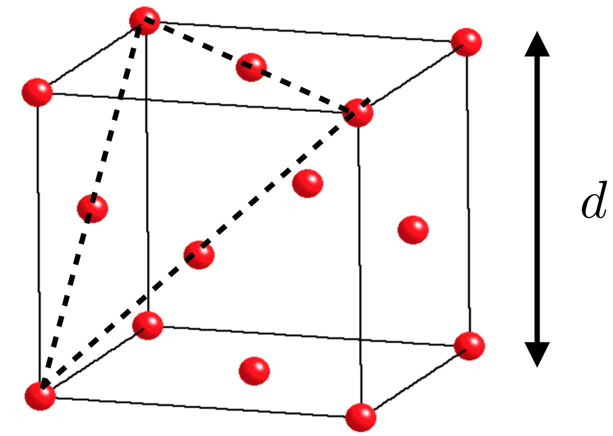
$$\alpha_i(\vec{r}_i(k)) = \tanh(\frac{\vec{r}_i(k).\vec{u}}{w})$$

$\vec{u}$ : unitary vector perpendicular to planes $(h_1k_1k_1)$

# S-PFM on FCC grid

## Why FCC grid ?

- maximise isotropy
- adapted to elastic solvers for discrete elastic fields




$\longrightarrow$ strategy for choosing  plane family $(h_1, k_1, l_1)$ :that receives continuous translational invariance :

- maximise the inter-reticular distance between planes  :  $(h_1 k_1 l_1) = (111)$

$\longrightarrow$ to minimise pinning along other directions !

$\longrightarrow$ for rotational invariance :

- select 2 other families :  $(h_2 k_2 l_2) = (200)$  and  $(h_3 k_3 l_3) = (220)$
- extend gradient terms up to 3rd neighbours
- optimisation procedure on the weighting terms  $\gamma_2$ and $\gamma_3$ of the gradient terms :

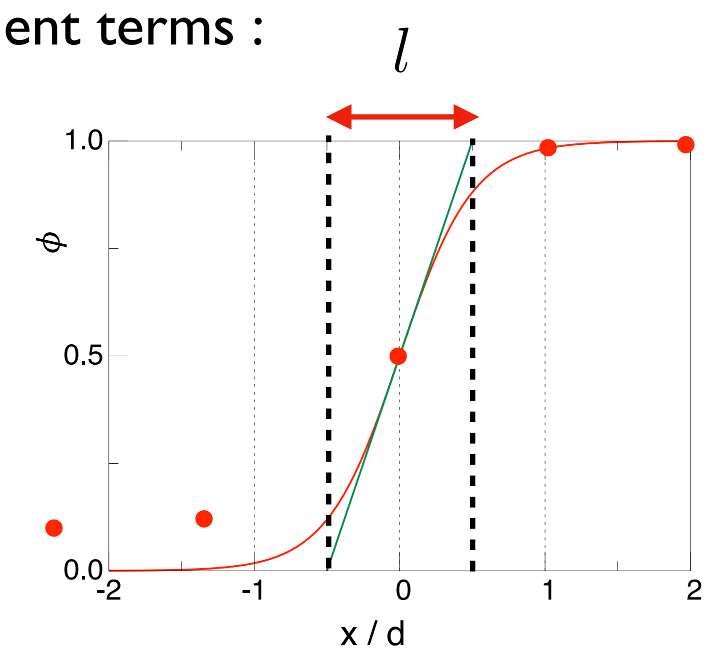
for $\boxed{\frac{l}{d} = \frac{2}{3}}$ $\longrightarrow$ we get :

| | |
|---|---|
| $\gamma_2$ | 0.1736 |
| $\gamma_3$ | 0.2545 |

| | |
|---|---|
| $\sigma(111)$ | 0.671991 |
| $\sigma(200)$ | 0.671989 |
| $\sigma(220)$ | 0.671990 |

(units: $\lambda d^{-2}$)

$$\boxed{\frac{\Delta\sigma}{\sigma} \simeq 2\,10^{-6}\ !}$$



# Quality of the S-PFM (1)

- growth of a single precipitate

free energy density

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

kinetics

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

$\Delta F > 0$

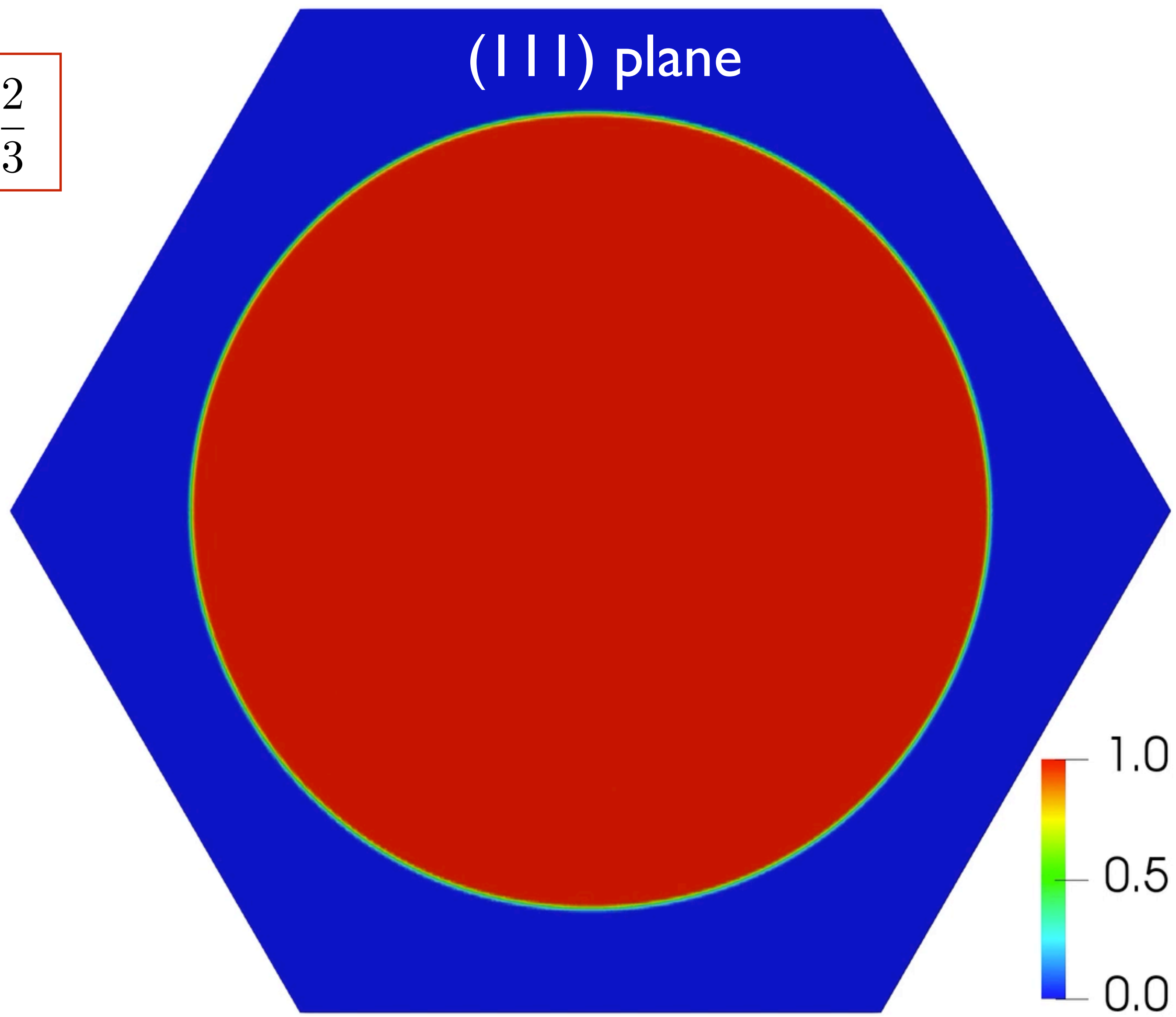
$h(\phi) = 3\phi^2 - 2\phi^3$

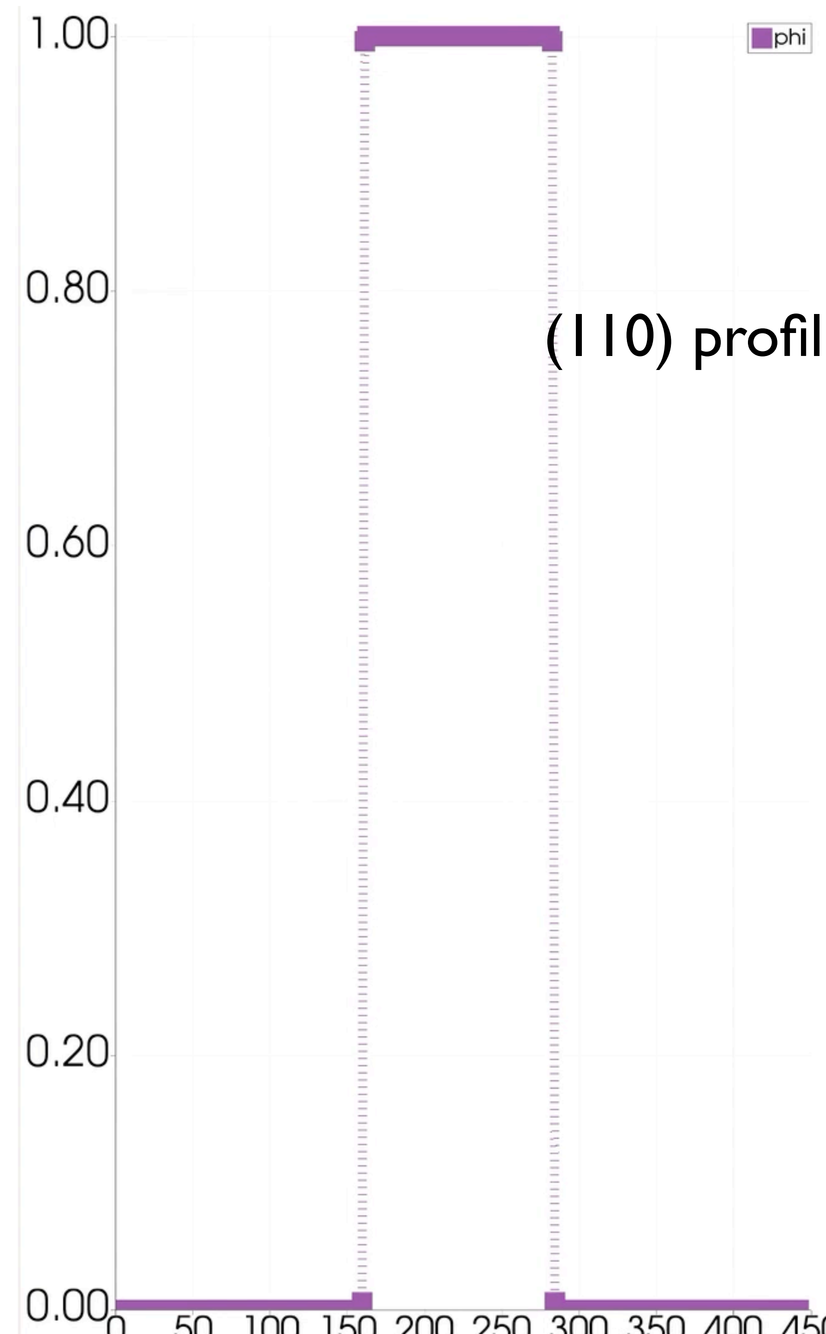
precipitate : $\phi = 1$

matrice : $\phi = 0$

- simulation : 256x256x256

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



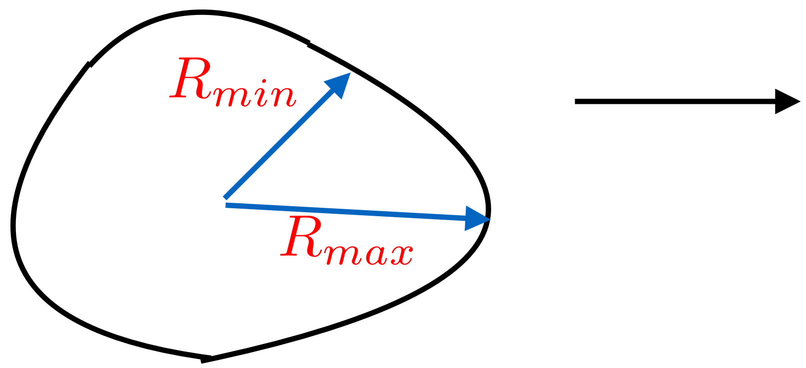



# Quality of the S-PFM (2)

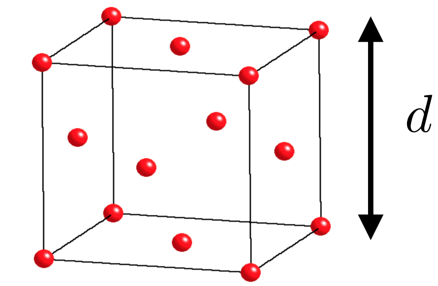
- Sphericity criteria to test the rotational invariance :

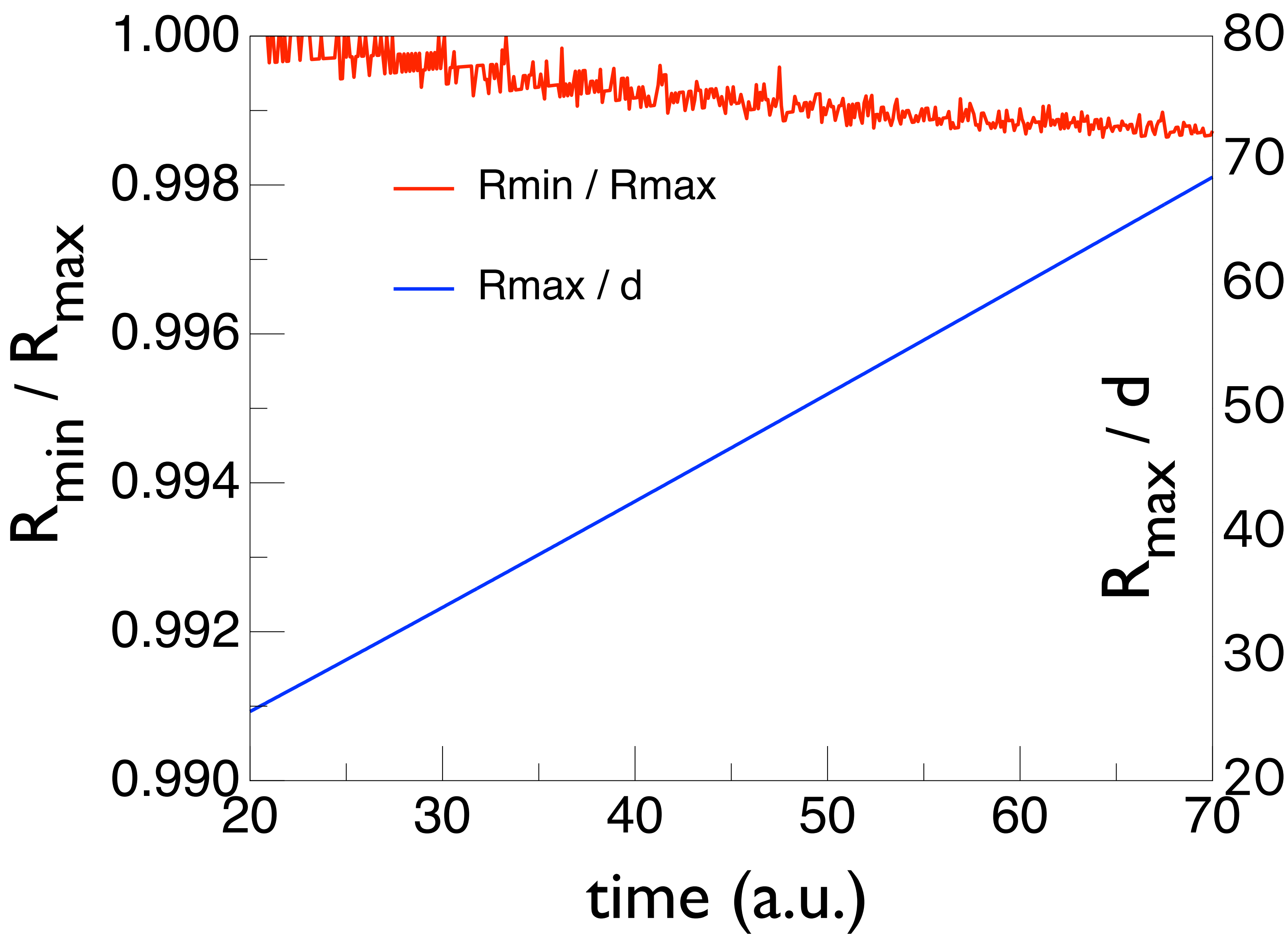
a growing precipitate :

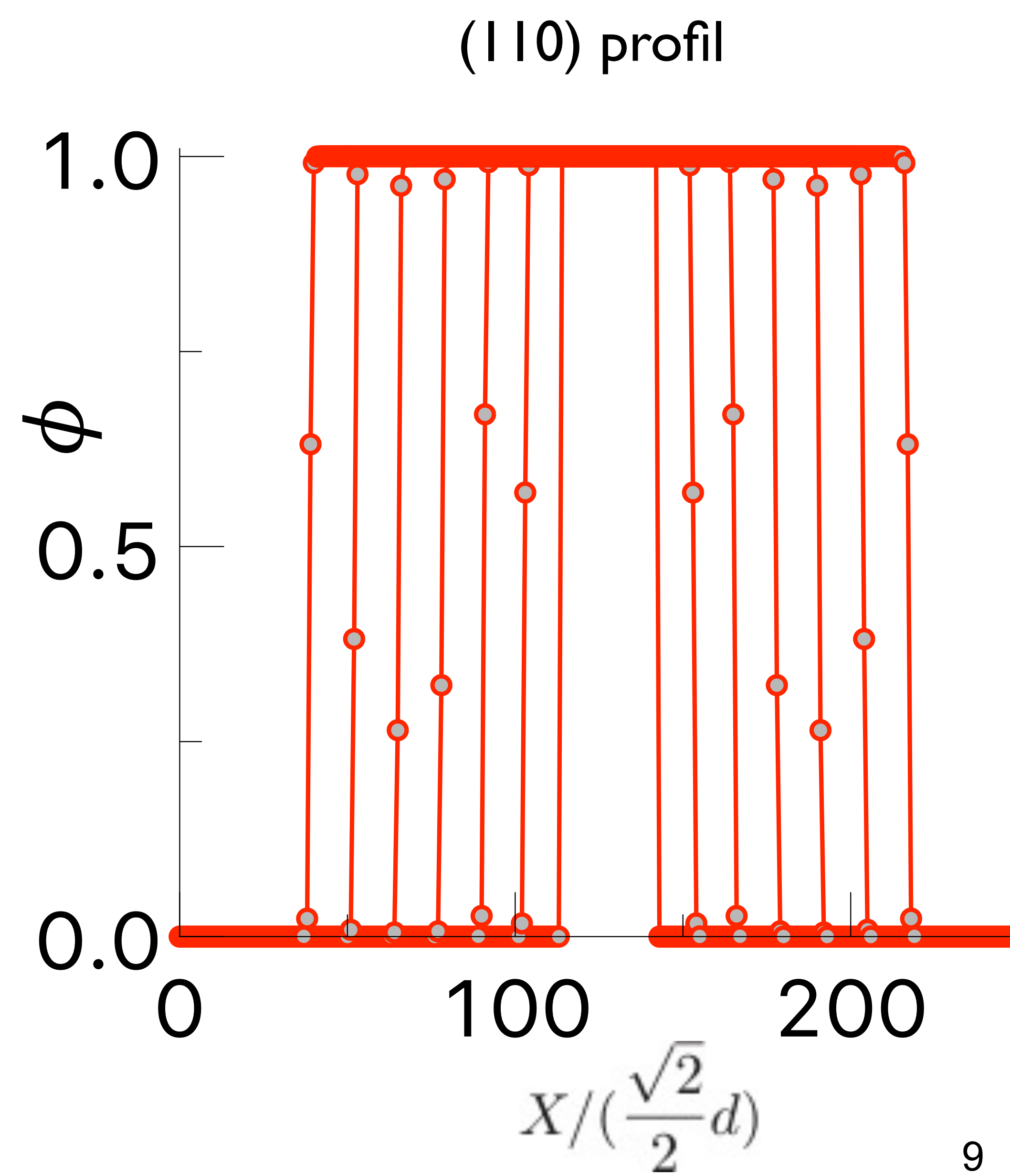
$$\frac{l}{d} = 1$$




$$\frac{R_{min}}{R_{max}}$$



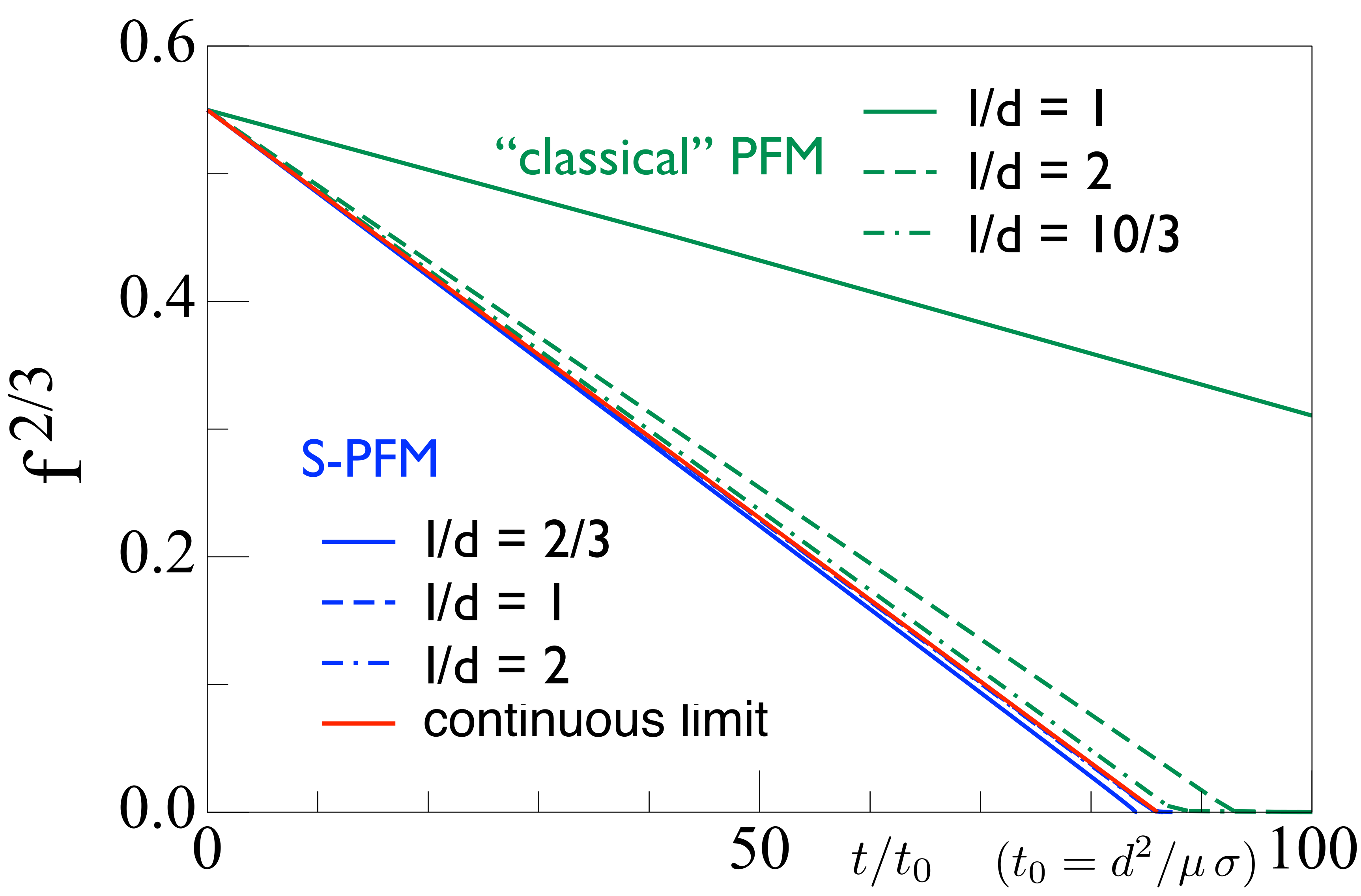



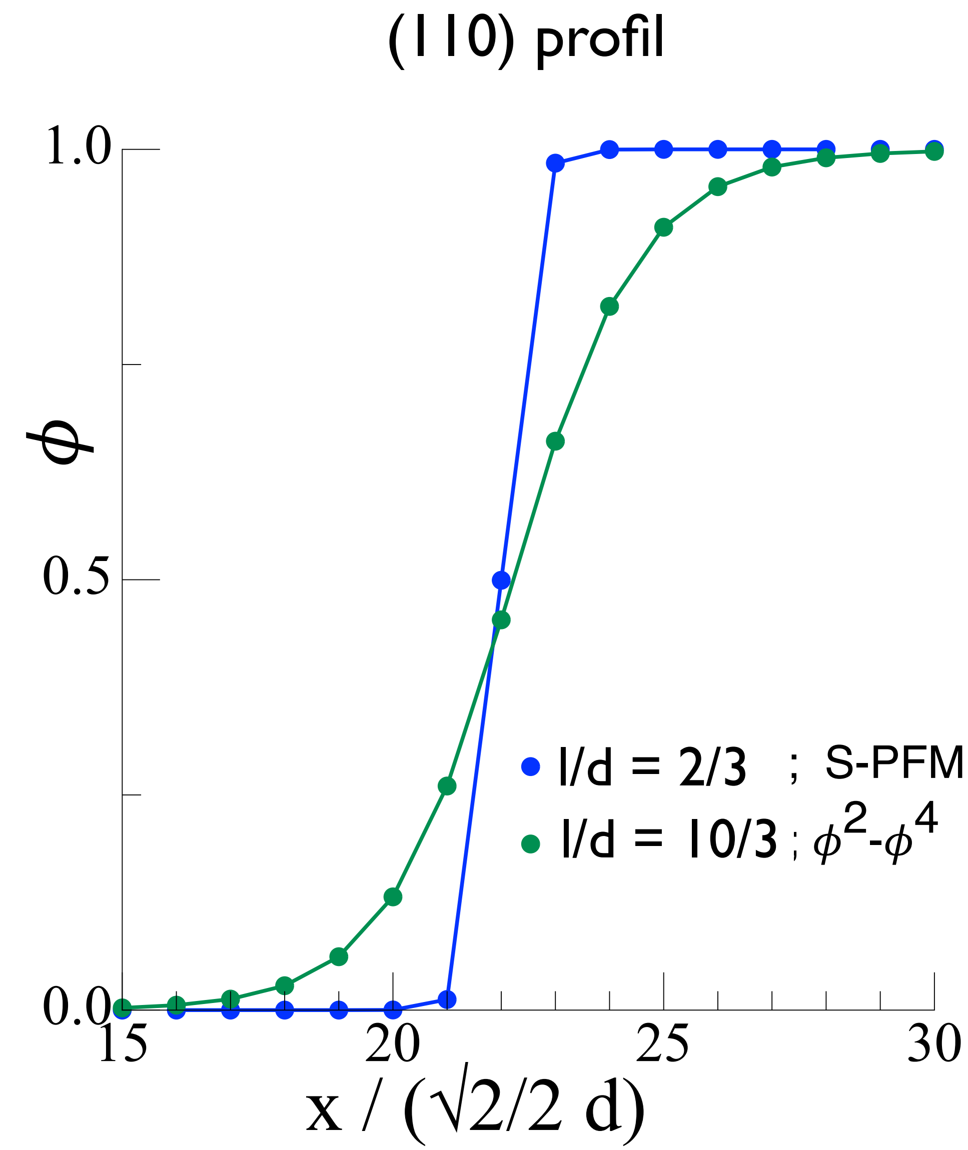
# Interfacial kinetic properties :

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 (concentration)

$\longrightarrow$ free energy density :

$$f(c,\phi) = g(\phi) + \frac{\lambda}{2}||\nabla_d \phi||^2 + f_{chem}(c,\phi,\nabla c) \qquad ||\nabla_d||^2 : \text{S-PFM extended gradient term}$$

$\longrightarrow$ kinetics :

$$\frac{\partial c}{\partial t} = M \nabla^2 \frac{\partial f_{chem}(c,\phi)}{\partial c}$$

$$\frac{\partial \phi}{\partial t} = -L\{g'(\phi) - \lambda \Delta_d \phi - \frac{\partial f_{chem}(c,\phi)}{\partial \phi}]\}$$

$\longrightarrow$ but :

- coupling between c and $\phi$ may play a rôle into the interface profil
- look for a $f_{chem}(c,\phi,\nabla c)$ such that a planar interface keeps the S-PFM interface profil even in c and $\phi$ are coupled !

$\longrightarrow$ solution :

$$f_{chem}(c,\phi) = h(\phi) f_1(c_1) + (1-h(\phi)) f_2(c_2)$$

$$c = h(\phi) c_1 + (1-h(\phi)) c_2$$

state variables : c and $\phi$

$$c = h(\phi) c_1 + (1-h(\phi)) c_2$$

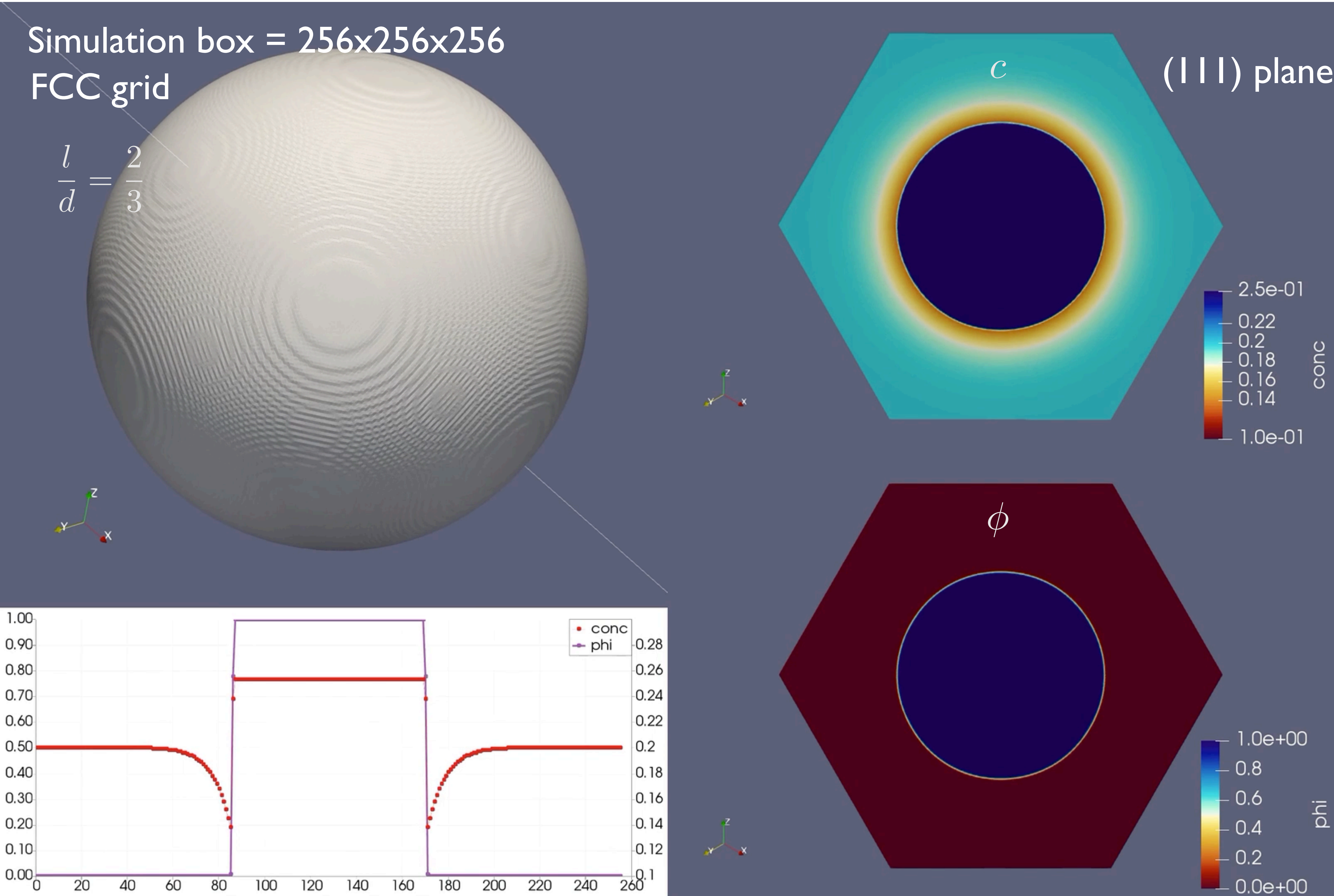
$$\frac{\partial f_1(c_1)}{\partial c_1} = \frac{\partial f_2(c_2)}{\partial c_2}$$

$\longrightarrow$

$$c_1 = c_1(c,\phi)$$

$$c_2 = c_2(c,\phi)$$

# S-PFM with a conserved order parameter



# S-PFM with a conserved order parameter and elastic fields

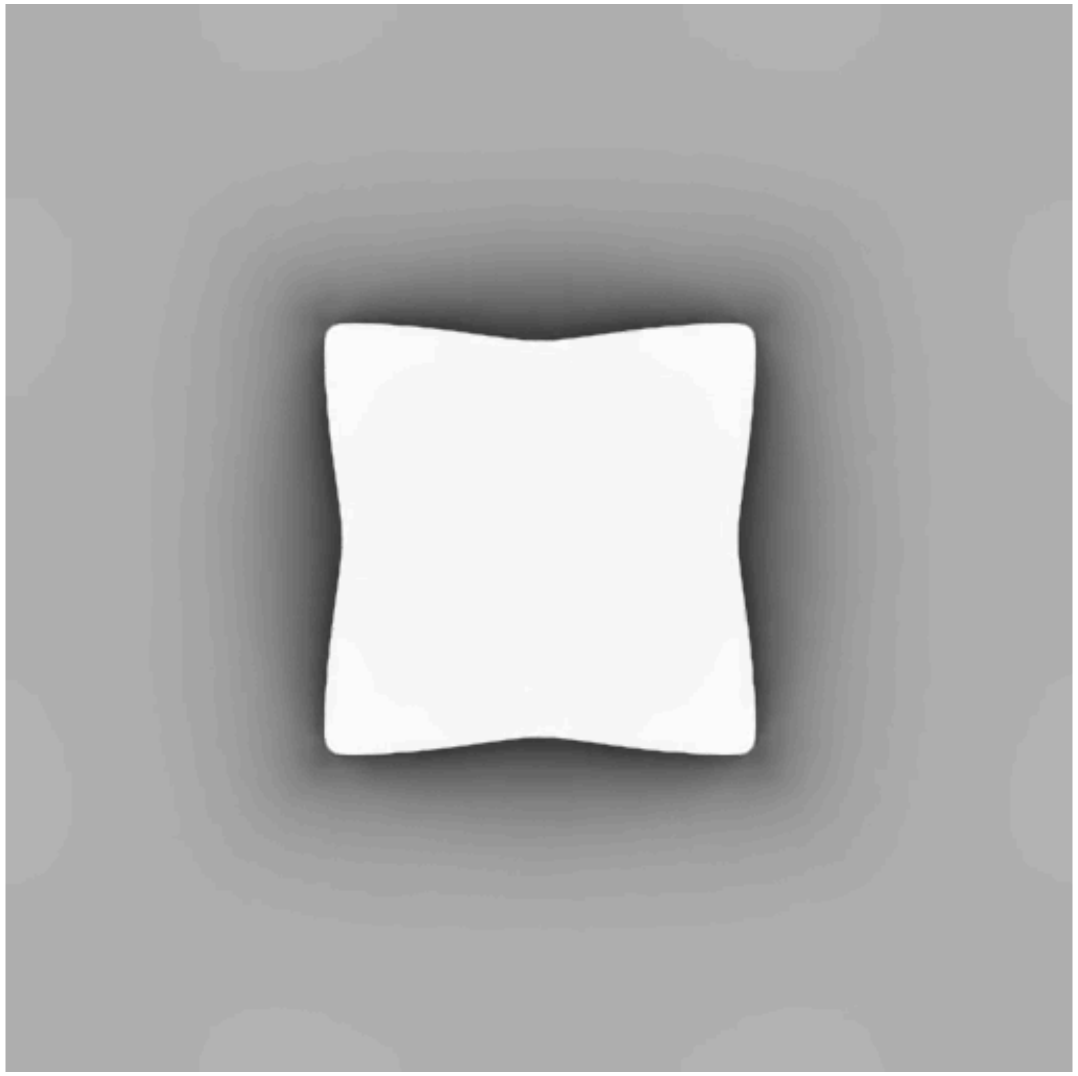
- Inhomogeneous elasticity :

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

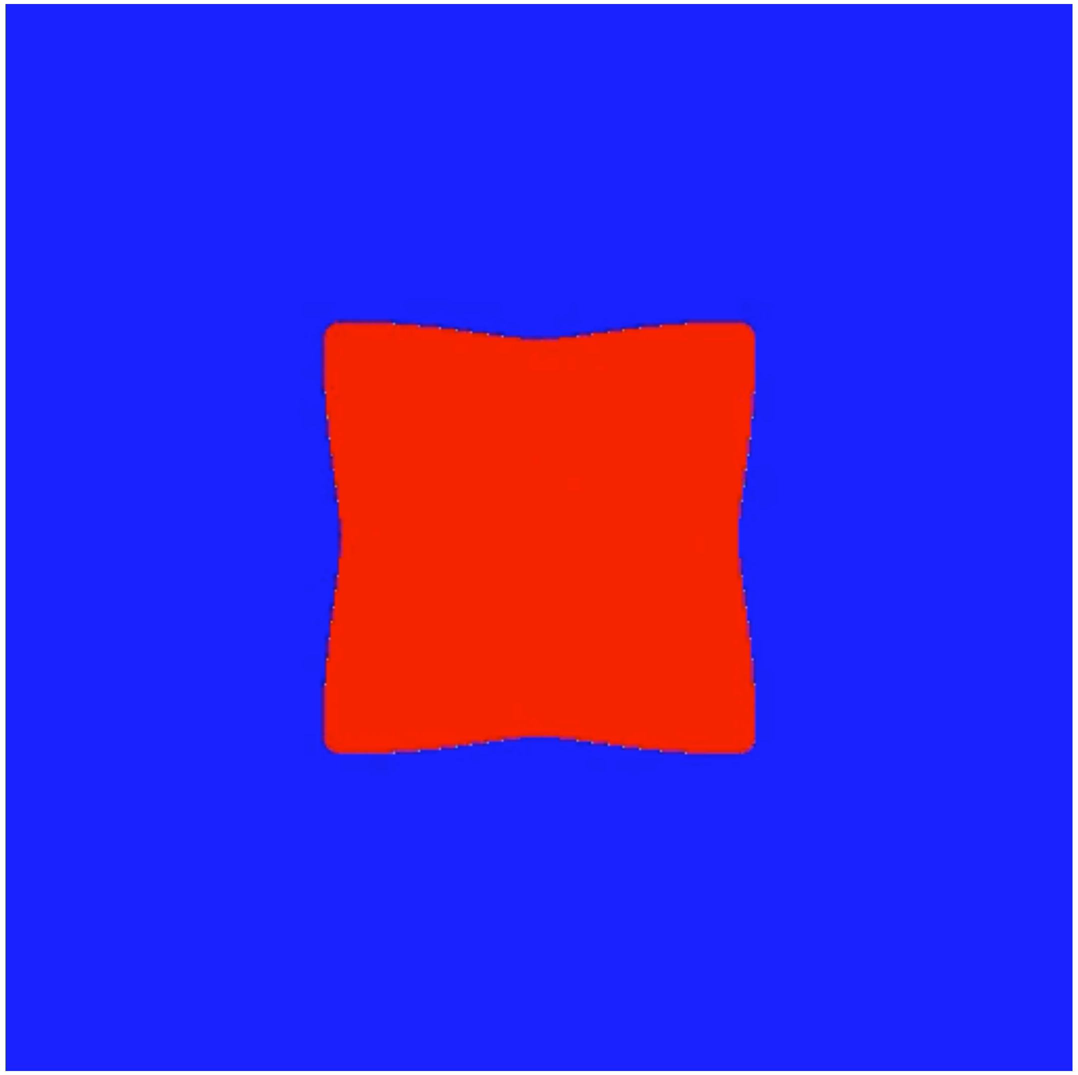
$$\gamma \quad \begin{aligned} C_{11} &= 197 \text{ GPa} \\ C_{12} &= 144 \text{ GPa} \\ C_{44} &= 90 \text{ GPa} \end{aligned}$$

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

concentration field

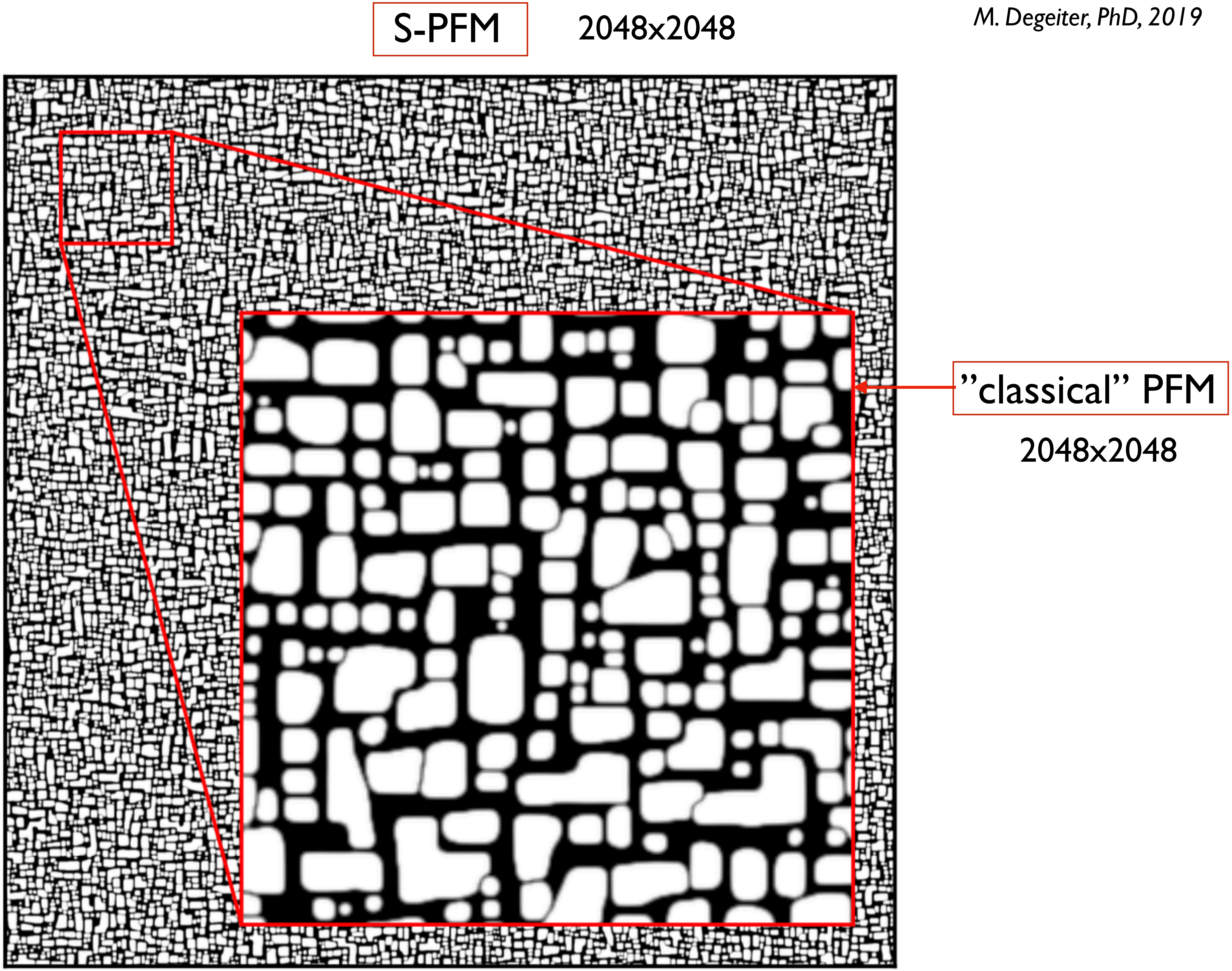


phase field



# Microstructures in Ni-based super-alloys

*M. Degeiter, PhD, 2019*



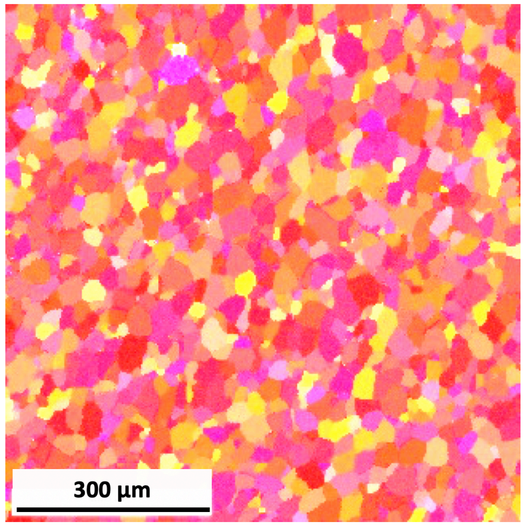
# S-PFM : a multi-phase field extension for polycristals (1)

## Grain growth by "classical" Phase Field Method

- nbr of grains in a representative stationary state : $N \sim 3\,10^4$
- nbr of initial grains needed to reach this stage : $N_0 \sim 3\,10^5$
- interface thickness << grain sizes : $l \sim D/10$
- grid step <<interface width : $d \sim l/10$

$\longrightarrow$ nbr of voxels $\sim 10^{12}$

Ni - 14%W ; 100 °C - 10 mn

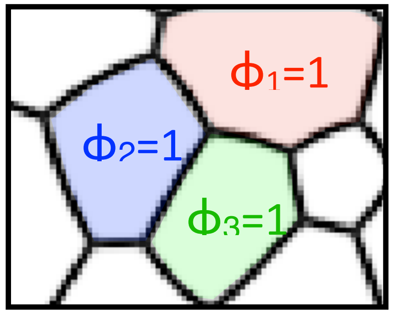



*Polycrystalline grain growth is one of the most important microstructure evolutions in engineering processes.*

## A multi-phase field S-PFM : *(Dimokrati et al, Acta Mat., 2020)*

$$F = V_d \sum_{\mathbf{r}} \Delta f \left[ \sum_i g(\phi_i) + \gamma \sum_{i>j} \phi_i^2 \phi_j^2 \right] + \frac{\kappa}{2} \sum_i |\nabla^d \phi_i|^2$$

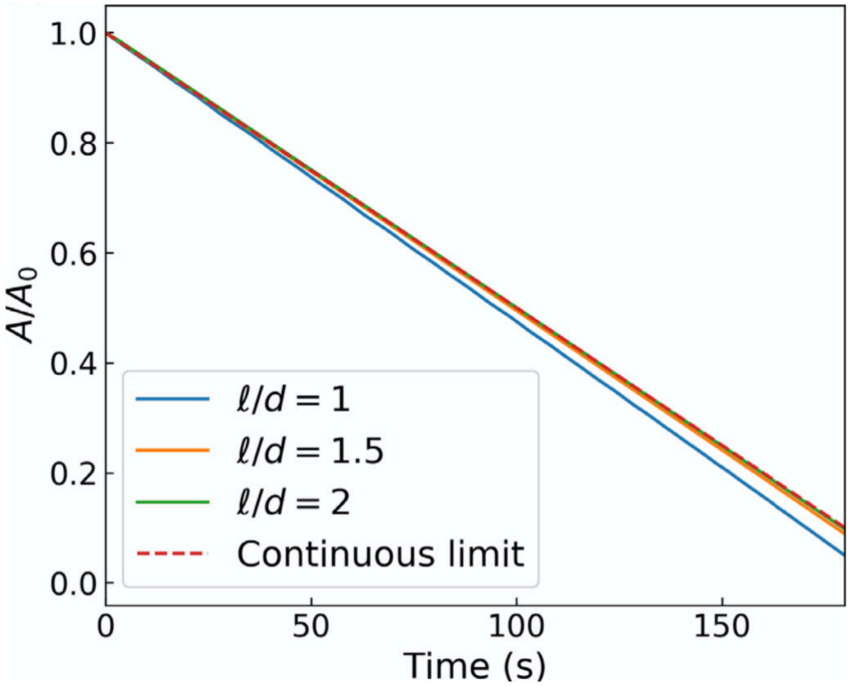
$$g(\phi) = -\frac{\phi^2}{4}(3\phi^2 - 8\phi + 6) + \frac{\kappa}{4\Delta f} \sum_s^{N_s} \frac{2\gamma_s}{m_x d_s^2} \sum_{k=1}^{m_s} \left[ \frac{\alpha_s^2(k) - 1}{\alpha_s^2(k)} ln\left[1 - \alpha_s^2(k)(2\phi - 1)^2\right] - (2\phi - 1)^2 \right]$$




## Collapse of a circular grain :

- square grid, grid step : $d$
- interface thickness : $l$

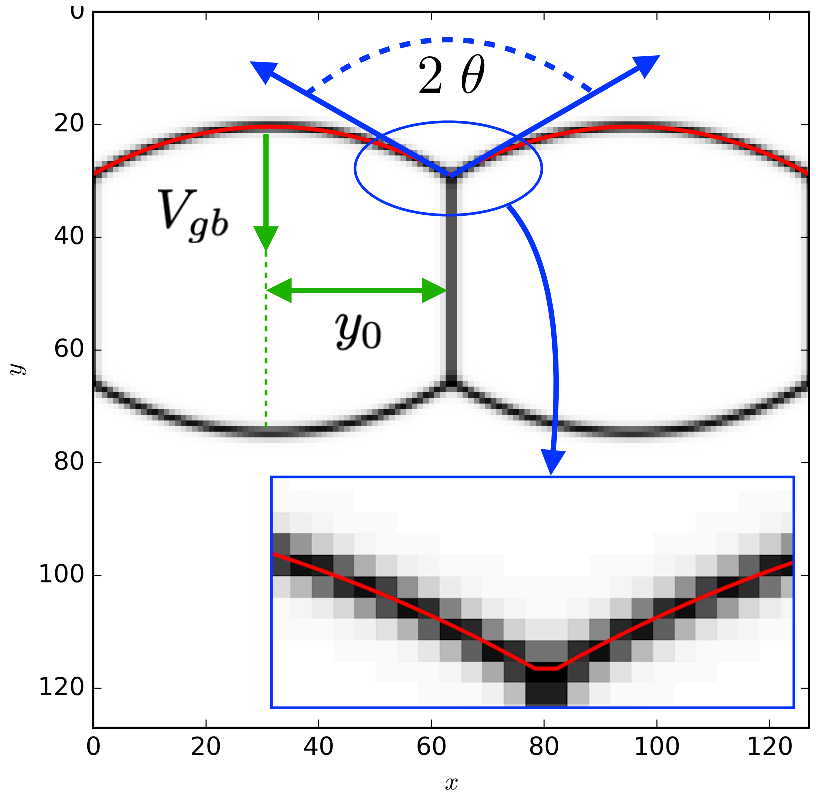
| $l/d$ | precision on slope |
|---|---|
| — 1 | 5.20 % |
| — 1.5 | 1.06 % |
| — 2 | 0.04 % |



# S-PFM : a multi-phase field extension for polycristals (2)

*(Dimokrati et al, Acta Mat., 2020)*

## Question : behaviour of triple junctions ?




simulation

theoretical shape :

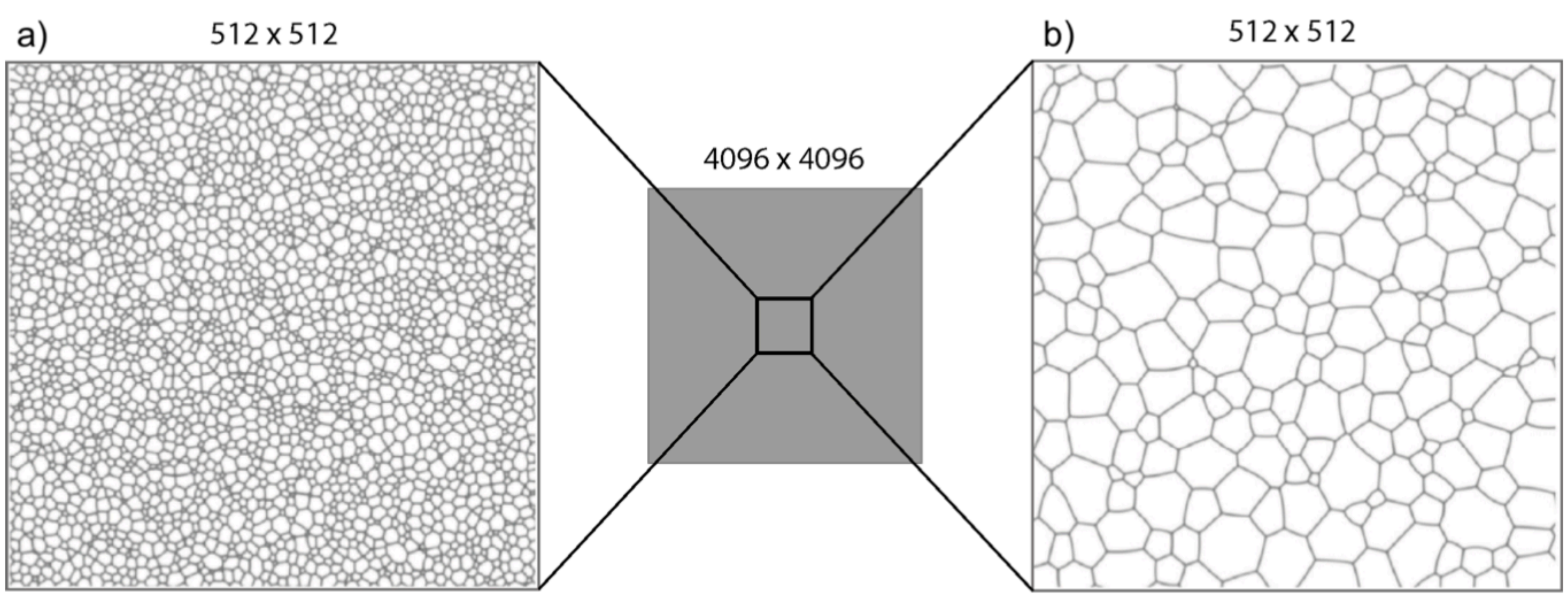
$$y(x) = y_0 \frac{\cos^{-1}(e^{-\frac{x}{y_0}\cos^{-1}\sin\theta})}{\cos^{-1}\sin\theta}$$

Triple junction properties
(when no junction drag)

| | theory | S-PFM |
|---|---|---|
| $\theta$ | $\pi/3$ | $60.25 \pm 0.25°$ |
| $V$ | $\pi/6$ (0.5236...) | 0.525 |

$(V\,units : m_{gb}\,\sigma_{gb}\,y_0^{-1})$

## Statistical analysis of grain size distribution :




$t/t_0 = 100$
$< R > = 7.9d \quad N = 166000$

$t/t_0 = 3000$
$< R > = 19.3d \quad N = 12400$