Adaptive finite elements with high aspect ratio for the computation of dendritic growth and coalescence in binary alloys.

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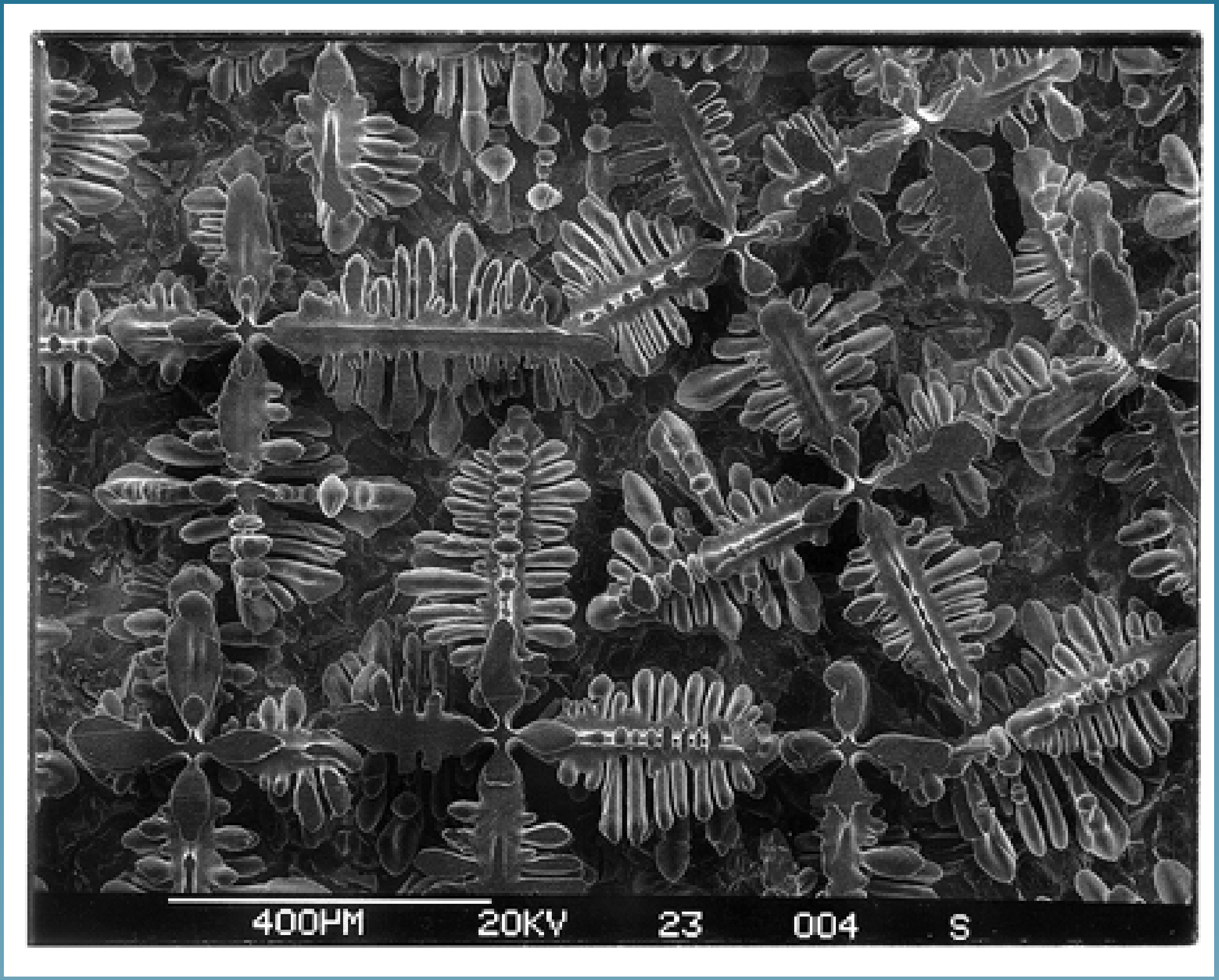
Outline

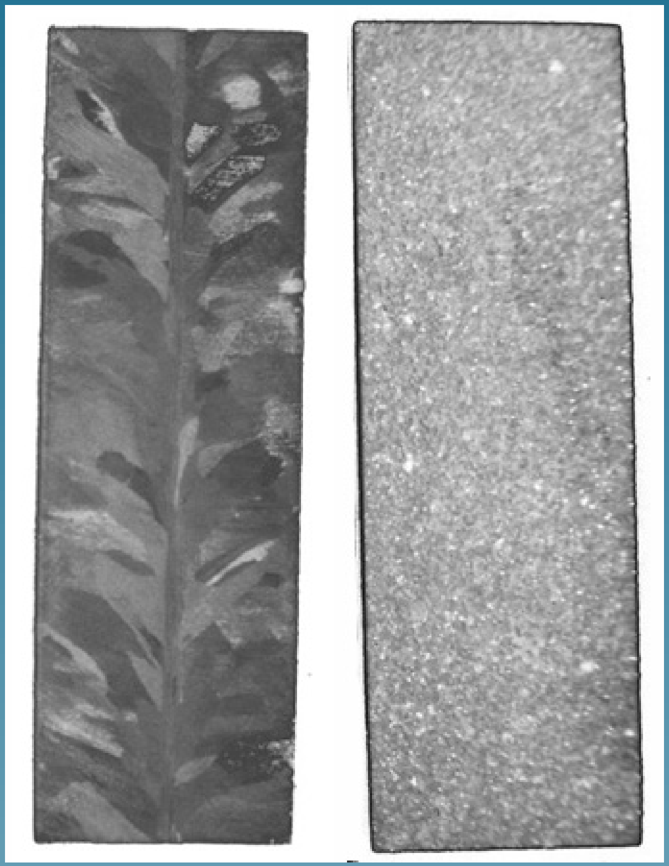
- A phase field model for dendritic growth of binary alloys
  - ⋆ Model
  - ⋆ Existence, a priori and a posteriori error estimates
  - ⋆ Numerical Tool : Adaptive finite elements with high aspect ratio
- A multiphase field model for the coalescence of binary alloys

Solidification : dendritic growth



Sa-Co alloy

Solidification : from macro to micro scale



Grain shape and size ($\longrightarrow$ mechanical properties) :

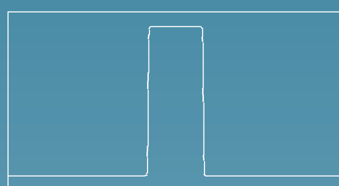
depend on solidification history

A phase field model for dendritic growth of a binary alloy

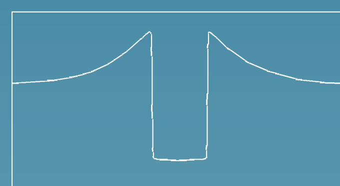
- Phase field model (Warren Boettinger Acta Metall. Mater. 1995, Tiaden Nestler Diepers Steinbach Phys D 1998). Find $c, \phi : \Omega \times (0,T) \rightarrow \mathbb{R}$ such that

$$\frac{\partial \phi}{\partial t} - \mathrm{div}\ (A(\nabla\phi)\nabla\phi)) \ - S(c,\phi) = 0 \qquad \text{in } \Omega \times (0,T),$$

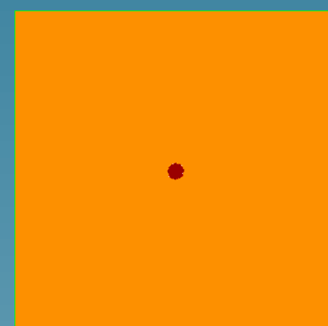
$$\frac{\partial c}{\partial t} - \mathrm{div}\ \Big(D_1(\phi)\nabla c + D_2(c,\phi)\nabla\phi\Big) = 0 \qquad \text{in } \Omega \times (0,T).$$



Phase field ϕ
$\phi = 0$: liquid
$\phi = 1$: solid



Concentration c



Initial time

Final time

- interface width : ε small $\simeq 10^{-8}\ m$ (100 atoms).

The phase field equation

- Phase field

$$\frac{\partial \phi}{\partial t} - \text{div}\,(A(\nabla\phi)\nabla\phi)\ \ - S(c,\phi) = 0.$$

- Free energy = interface (anisotropy) + double wells + phase transformation

$$\frac{\varepsilon}{2}\int_\Omega a^2(\theta(\nabla\phi))|\nabla\phi|^2 + \frac{1}{\varepsilon}\int_\Omega W(\phi) + \int_\Omega c_\ell - c_\ell^{eq},$$

  with $a(\theta) = (1 + \bar{a}\cos(\kappa\theta))$ and $\theta(\nabla\phi)$ angle between $\nabla\phi$ and horizontal.

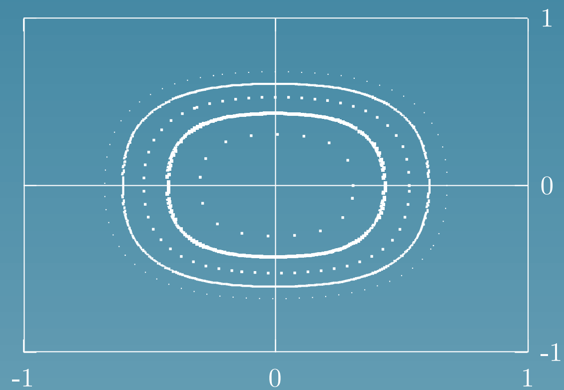
- Small parameter in $S(c,\phi)$ (time step $\simeq \varepsilon^2$, Elliott State of the art in numer. anal. 1997), strongly nonlinear div $(A(\nabla\phi)\nabla\phi)$.

- Existence for low physical anisotropy $\bar{a} < \frac{1}{\kappa^2-1}$, a priori error estimates (Burman Rappaz M3AS 2003).

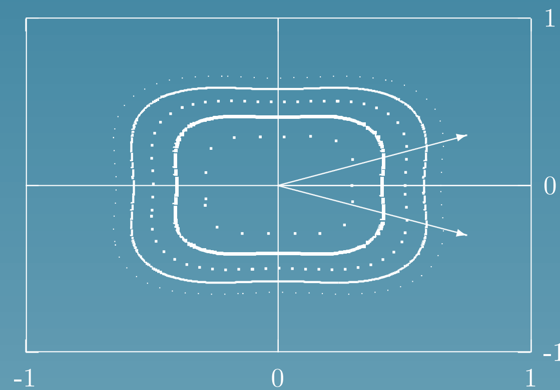
- A posteriori error estimates, adaptive FE with high aspect ratio (Burman Picasso J. Interfaces Free Boundaries 2003).

Small and large physical anisotropy

- Interface energy $\int_\Omega a^2(\theta(\nabla\phi))|\nabla\phi|^2$.
- $a(\theta) = (1 + \bar{a}\cos(\kappa\theta))$ and $\theta(\nabla\phi)$ angle between $\nabla\phi$ and horizontal.
- isolines of $\xi \to a^2(\theta(\xi))|\xi|^2$



Small physical anisotropy $\bar{a} < \frac{1}{\kappa^2 - 1}$



Large physical anisotropy $\bar{a} > \frac{1}{\kappa^2 - 1}$

A posteriori error estimates, adaptive FE with high aspect ratio

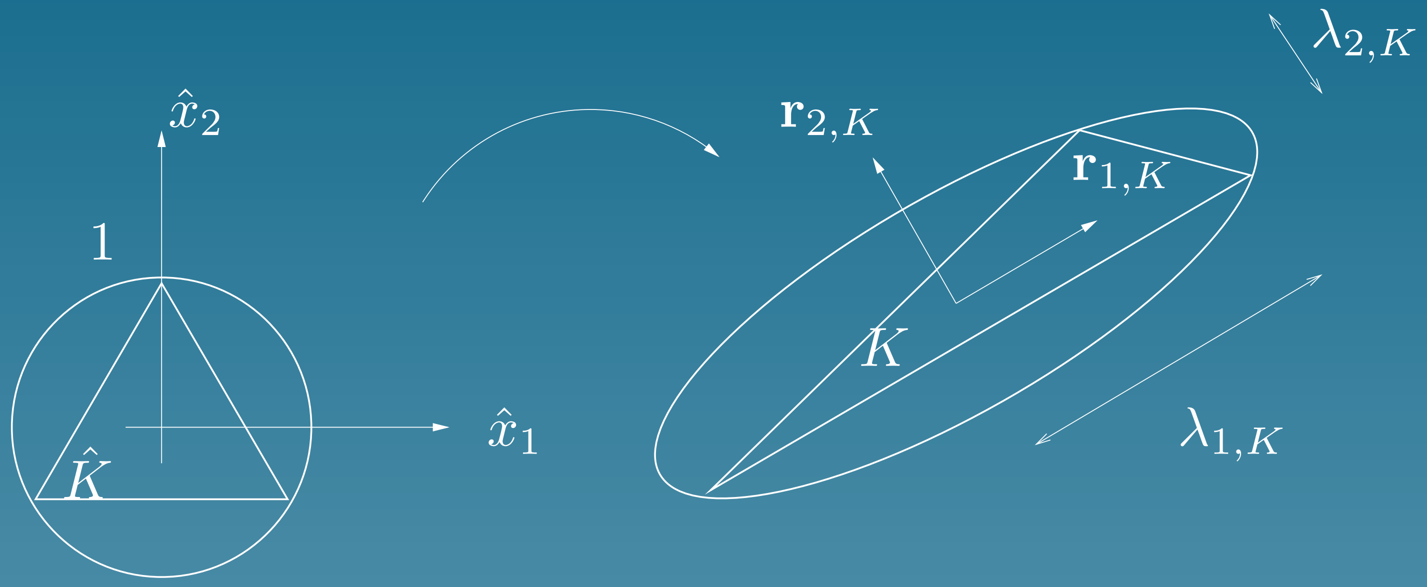
- A posteriori error estimates : error $\leq$ estimator(mesh,numerical solution).
- $A(\cdot)$ is strongly elliptic : $\bar{a} < \frac{1}{\kappa^2-1}$, $\exists \mu$

$$\mu \int_\Omega |\nabla(\phi-\psi)|^2 \leq \int_\Omega \Big(A(\nabla\phi)\nabla\phi - A(\nabla\psi)\nabla\psi \Big) \cdot \nabla(\phi-\psi) \qquad \forall \phi, \psi \in H_0^1(\Omega).$$

- The error in the $L^2(0,T;L^2(\Omega))$ norm converges faster to zero than the error in the $L^2(0,T;H^1(\Omega))$ norm.
- Then, $\exists C$ independent of "everything" (problem data, mesh size and aspect ratio) such that

$$\mu \int_0^T \int_\Omega |\nabla(\phi-\phi_h)|^2 + \frac{\mu D_1^2}{D_2^2} \int_0^T \int_\Omega |\nabla(c-c_h)|^2$$
$$\leq C \left(est_\phi(mesh, \phi_h, c_h) + \frac{\mu D_1^2}{D_2^2} est_c(mesh, \phi_h, c_h) \right).$$

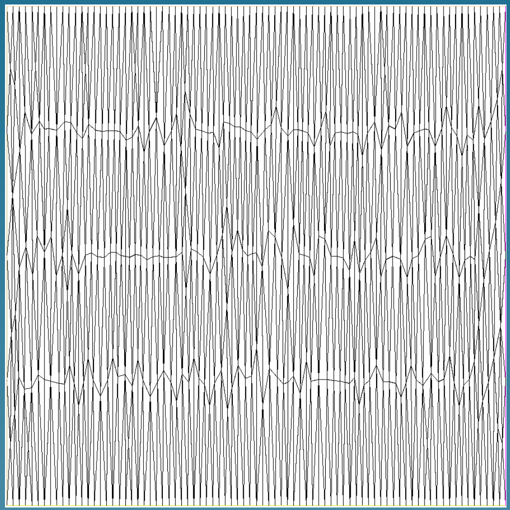
Error indicator for meshes with high aspect ratio



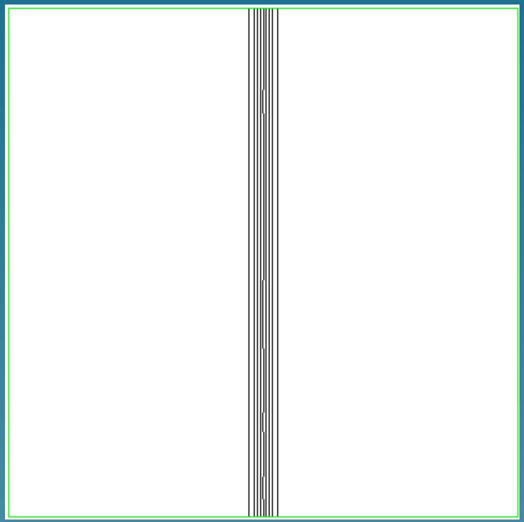
$$\frac{1}{2\lambda_{2,K}^{1/2}}\left\|\left[\frac{\partial c_h}{\partial n}\right]\right\|_{L^2(\partial K)}\left(\lambda_{1,K}^2\left(\mathbf{r}_{1,K}^T G_K(c-c_h)\mathbf{r}_{1,K}\right)+\lambda_{2,K}^2\left(\mathbf{r}_{2,K}^T G_K(c-c_h)\mathbf{r}_{2,K}\right)\right)^{1/2}$$

where $G_K(\cdot)$ is the matrix of first order derivatives, approached using post-processing techniques (Picasso SISC 2003).

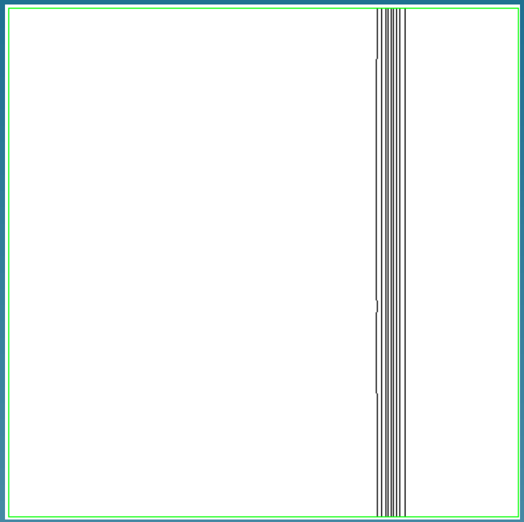
Numerical validation of the error indicator



mesh



ϕ, c at initial time



ϕ, c at final time

$h1 - h2$	e_{L^2}	e_{H^1}	ei^{ZZ}	ei^{A}
$0.000005 - 0.0001$	$1.1\ 10^{-6}$	0.29	1.01	1.85
$0.0000025 - 0.00005$	$3.2\ 10^{-7}$	0.13	1.01	1.74
$0.00000125 - 0.000025$	$8.8\ 10^{-8}$	0.066	1.01	1.74

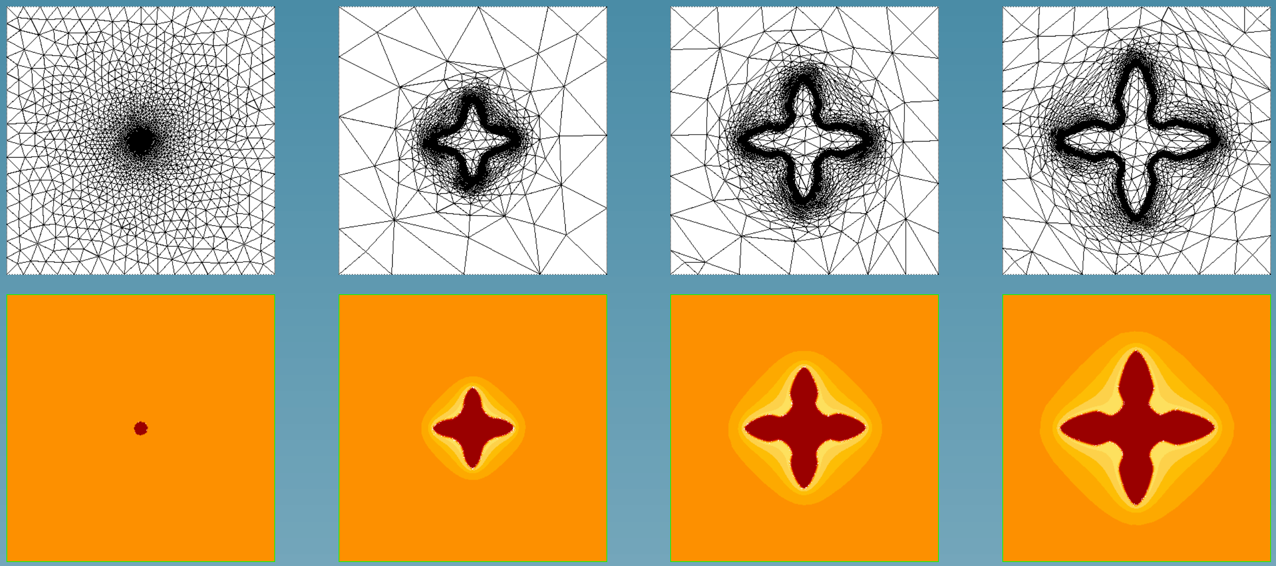
ei : effectivity index, error indicator / true error.

Small physical anisotropy

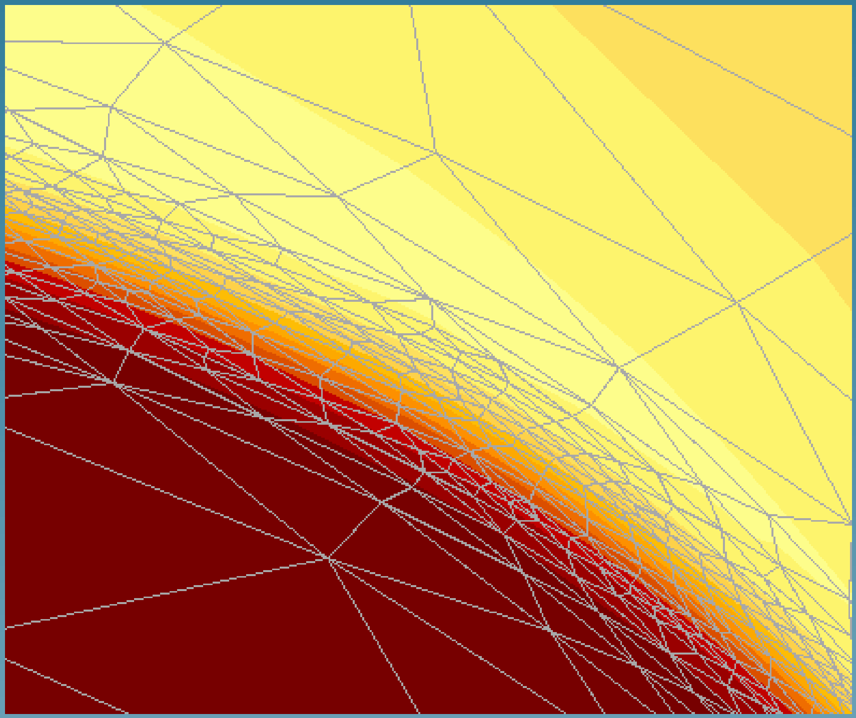
- Goal of the adaptive algorithm : build a sequence of triangulations such that

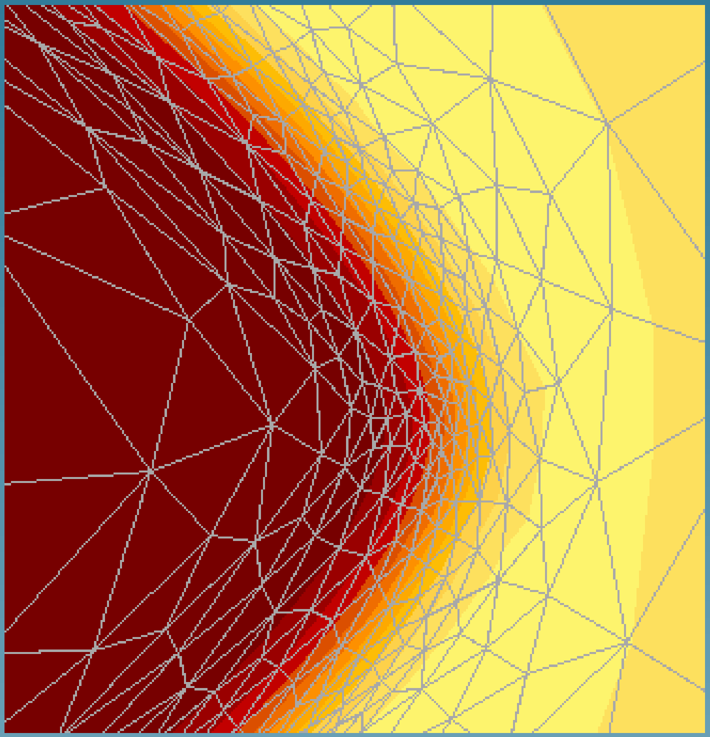
$$\frac{\text{error indicator}}{\int_0^T \int_\Omega |\nabla c_h|^2} \simeq TOL.$$

- Box width $5\ 10^{-4}$, $\varepsilon = 5\ 10^{-7}$, time step $5\ 10^{-4}$, $TOL = 0.0625$, 24000 vertices, final time 1.



Small physical anisotropy





Same precision with isotropic meshes : 10 times more vertices !

Convergence

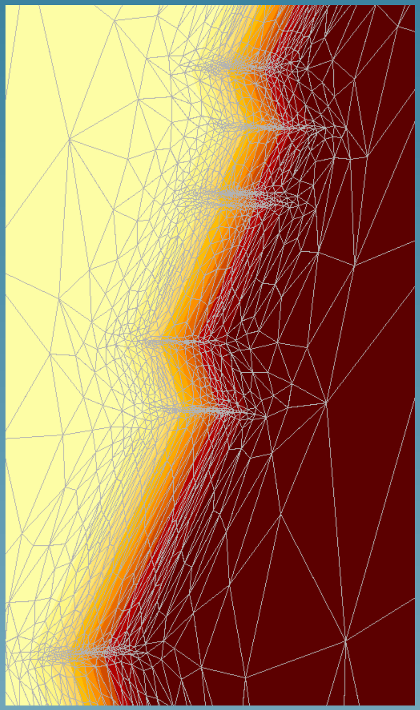
TOL=0.25
1987 Vertices

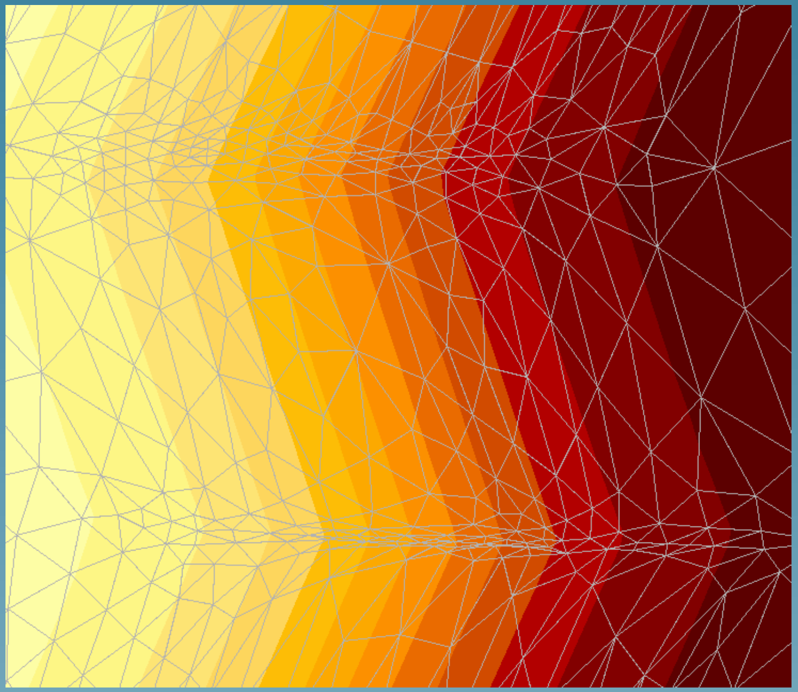
TOL=0.125
6073 Vertices

TOL=0.0625
24441 Vertices

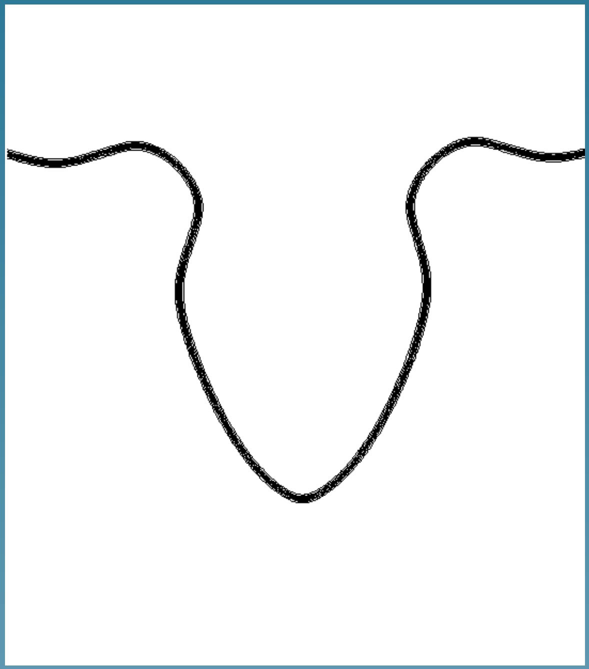
TOL=0.03125
101782 Vertices

Large physical anisotropy

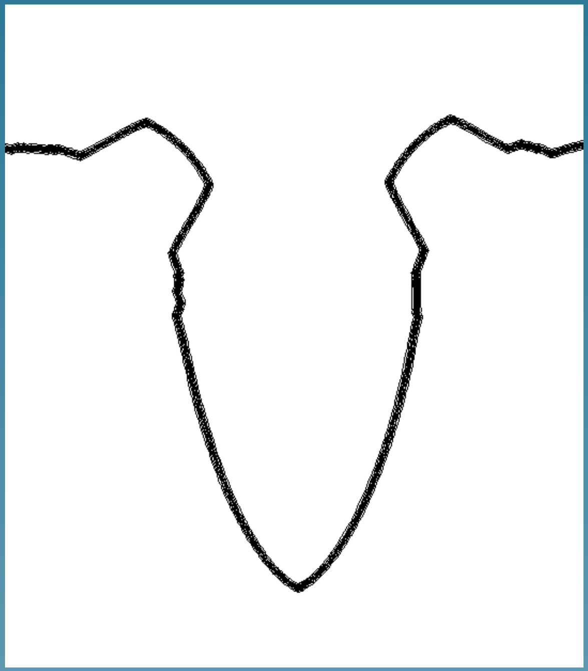




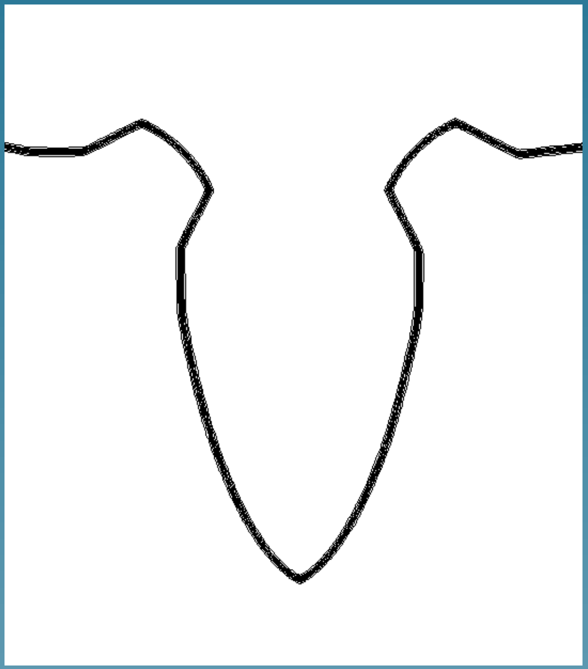
ϕ isolines according to physical anisotropy



Low anisotropy

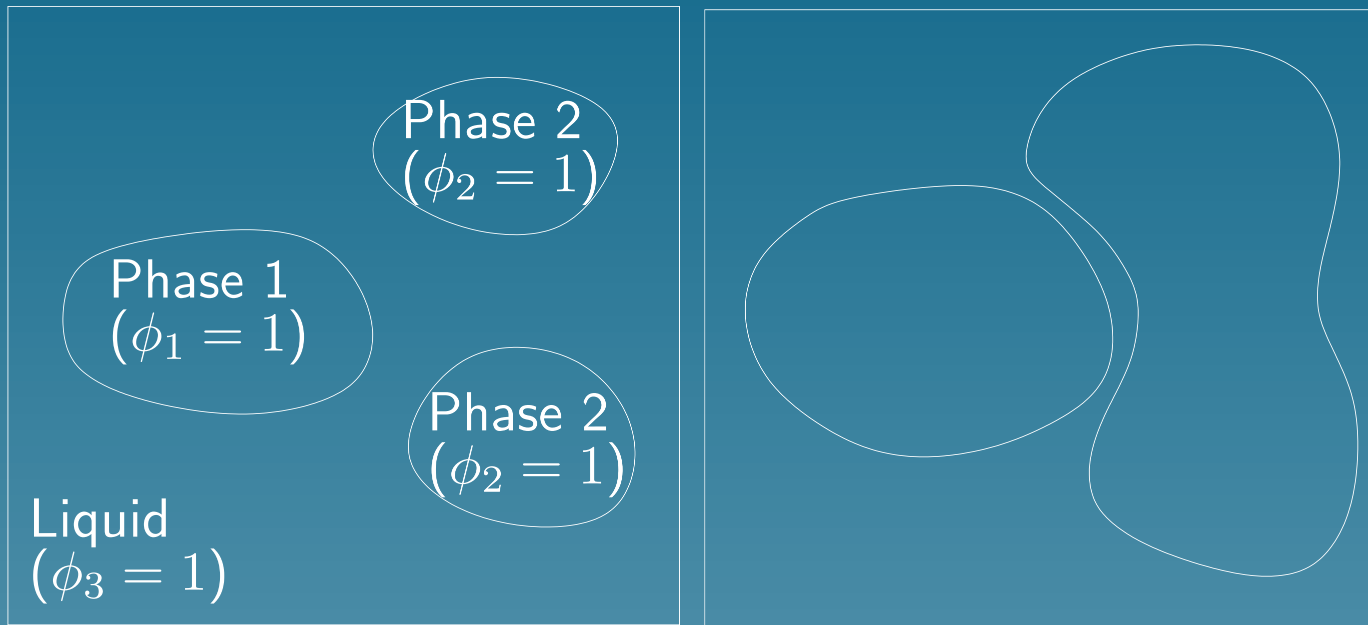


High anisotropy



High anisotropy
convexified functional

A multiphase field model for coalescence in binary alloys



- Multiphase field : Tiaden Nestler Diepers Steinbach Phys D 1998
- Multiphase field for binary alloys : Rappaz Jacot Boettinger Met. Trans. A 2003, Burman Jacot Picasso J. Comp. Phys. 2004
- Unknowns : ϕ_1, ϕ_2, ϕ_3, λ (Lagrange multiplier $\phi_1 + \phi_2 + \phi_3 = 1$) and c.

Free energy

- Interface energy

$$J_{int}(\phi_1,\phi_2,\phi_3) = \frac{\varepsilon_{12}^2}{2}\int_\Omega a^2\Big(\theta_{12}\big(\mathbf{r}(\phi_1,\phi_2)\big)\Big)|\mathbf{r}(\phi_1,\phi_2)|^2 + \frac{\varepsilon_{13}^2}{2}\int_\Omega a^2\Big(\theta_{13}\big(\mathbf{r}(\phi_1,\phi_3)\big)\Big)|\mathbf{r}(\phi_1,\phi_3)|^2 + \frac{\varepsilon_{23}^2}{2}\int_\Omega a^2\Big(\theta_{23}\big(\mathbf{r}(\phi_2,\phi_3)\big)\Big)|\mathbf{r}(\phi_2,\phi_3)|^2$$

where $\mathbf{r}(\phi_i,\phi_j) = \phi_i\nabla\phi_j - \phi_j\nabla\phi_i \qquad (i,j)\in\{(1,2),(1,3),(2,3)\}$

- Phase transformation $J_{tr}(\phi_1,\phi_2,\phi_3) = \int_\Omega (c_\ell - c_\ell^{eq})$

- Double wells $J_{dw}(\phi_1,\phi_2,\phi_3) = \dfrac{1}{\varepsilon}\int_\Omega \phi_1^2\phi_2^2 + \phi_1^2\phi_3^2 + \phi_2^2\phi_3^2$

The parabolic system of equations

- Find ϕ_1, ϕ_2, ϕ_3 such that $J_{int} + J_{tr} + J_{dw}$=min and $\phi_1 + \phi_2 + \phi_3 = 1$

- Lagrangian

$$\mathcal{L}(\phi_1, \phi_2, \phi_3, \lambda) = (J_{int} + J_{tr} + J_{dw})(\phi_1, \phi_2, \phi_3) + \int_\Omega \lambda(\phi_1 + \phi_2 + \phi_3 - 1).$$

- $\mathcal{D}\mathcal{L}(\phi_1, \phi_2, \phi_3, \lambda) = 0$

- Find ϕ_1, ϕ_2, ϕ_3, λ such that

$$\begin{aligned}
&\frac{\partial \phi_1}{\partial t} + \mathcal{D}_{\phi_1}\mathcal{L}(\phi_1, \phi_2, \phi_3, \lambda) = 0,\\
&\frac{\partial \phi_2}{\partial t} + \mathcal{D}_{\phi_2}\mathcal{L}(\phi_1, \phi_2, \phi_3, \lambda) = 0,\\
&\frac{\partial \phi_3}{\partial t} + \mathcal{D}_{\phi_3}\mathcal{L}(\phi_1, \phi_2, \phi_3, \lambda) = 0,\\
&\phi_1 + \phi_2 + \phi_3 - 1 = 0.
\end{aligned}$$

The parabolic system of equations

- Weak formulation with no anisotropy

$$\int_\Omega \Bigg(\begin{pmatrix} \frac{\partial \phi_1}{\partial t} \\ \frac{\partial \phi_2}{\partial t} \\ \frac{\partial \phi_3}{\partial t} \end{pmatrix} \cdot \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} + \begin{pmatrix} (\phi_2^2 + \phi_3^2) I_2 & -\phi_1\phi_2 I_2 & -\phi_1\phi_3 I_2 \\ & \dots & \\ & \dots & \end{pmatrix} \begin{pmatrix} \nabla\phi_1 \\ \nabla\phi_2 \\ \nabla\phi_3 \end{pmatrix} \cdot \begin{pmatrix} \nabla\psi_1 \\ \nabla\psi_2 \\ \nabla\psi_3 \end{pmatrix}$$

$$+ \begin{pmatrix} |\nabla\phi_2|^2 + |\nabla\phi_3|^2 & -\nabla\phi_1 \cdot \nabla\phi_2 & -\nabla\phi_1 \cdot \nabla\phi_3 \\ \dots & & \\ \dots & & \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{pmatrix} \cdot \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix}$$

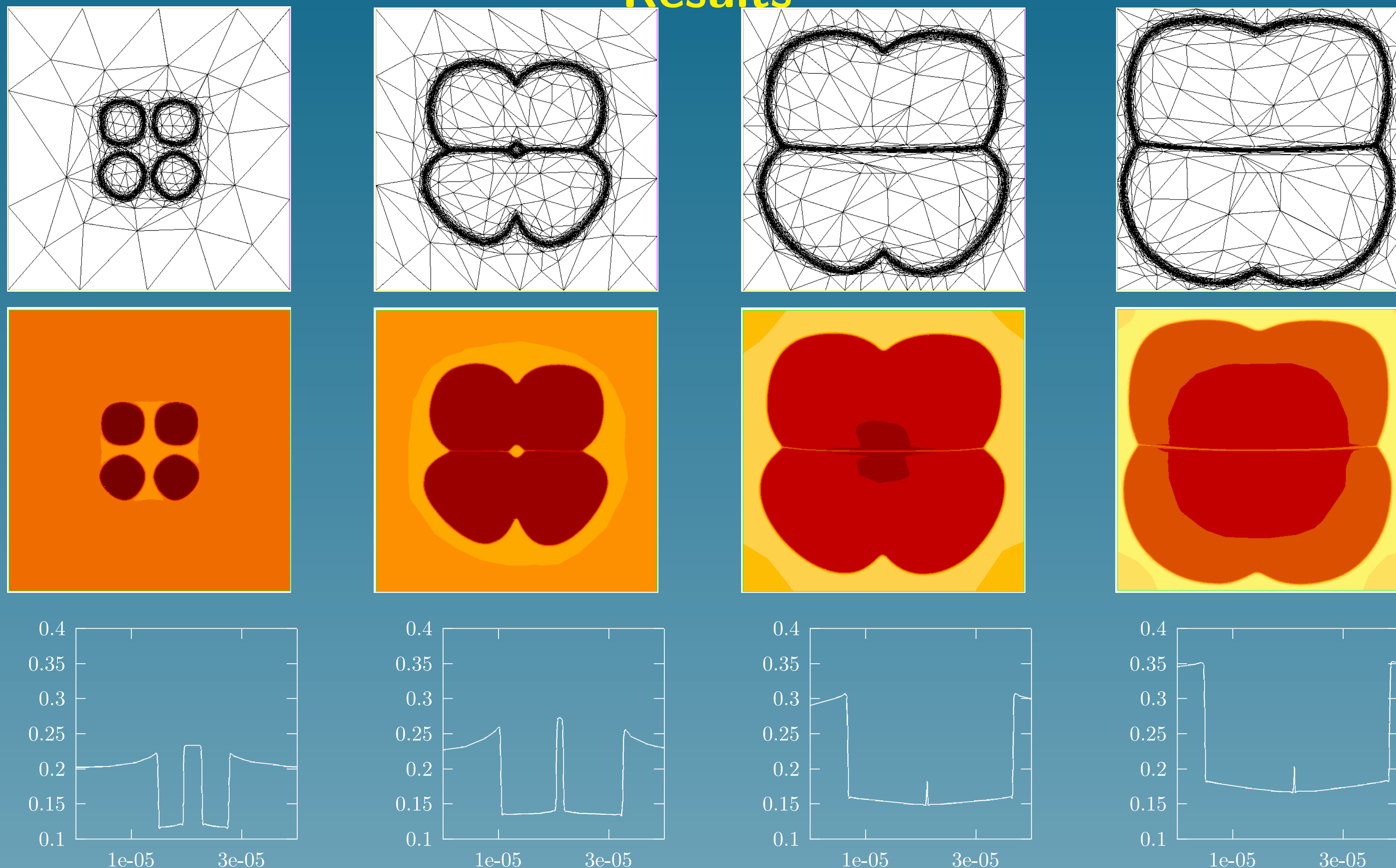
$$+ \text{double well stuff} + \lambda(\psi_1 + \psi_2 + \psi_3) \Bigg) = 0,$$

for all ψ_1, ψ_2, ψ_3.

$$\int_\Omega (\phi_1 + \phi_2 + \phi_3)\mu = \int_\Omega \mu,$$

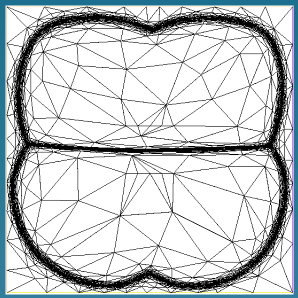
for all μ.

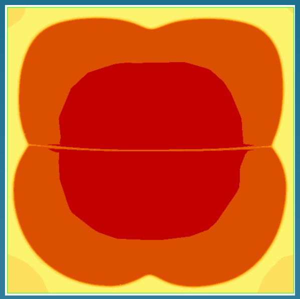
Results

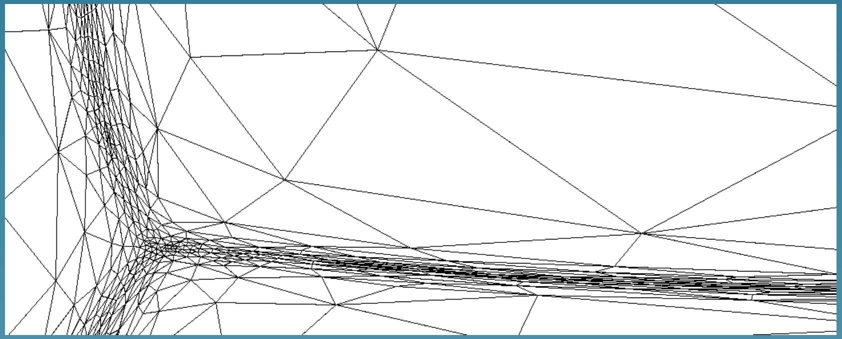


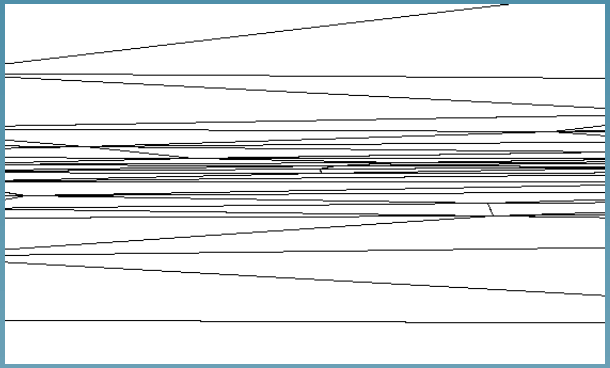
Box $3\ 10^{-5}$, $\varepsilon = 5\ 10^{-8}$, time step 10^{-3}, $TOL = 0.25$, 3000 vertices time 2.

Results

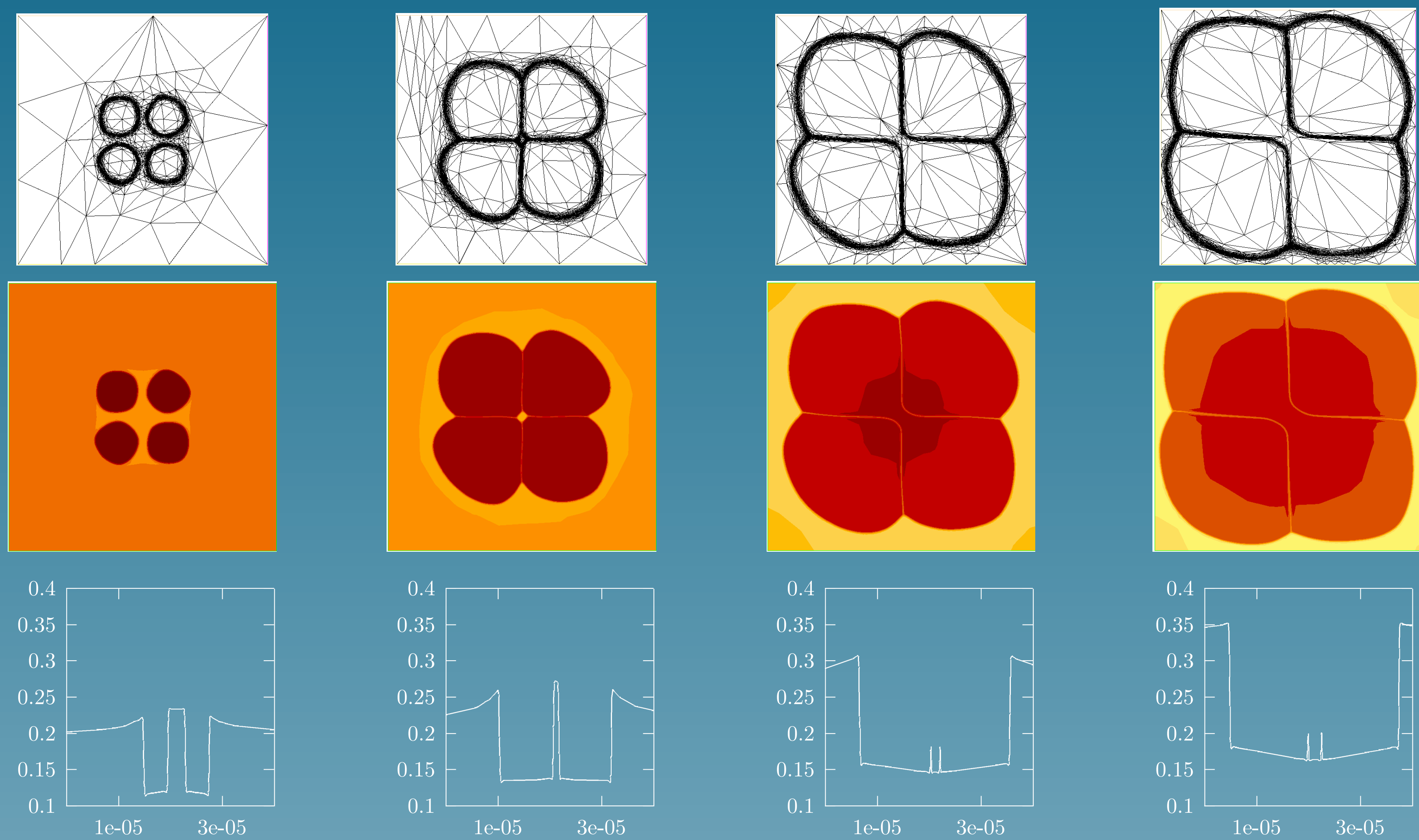








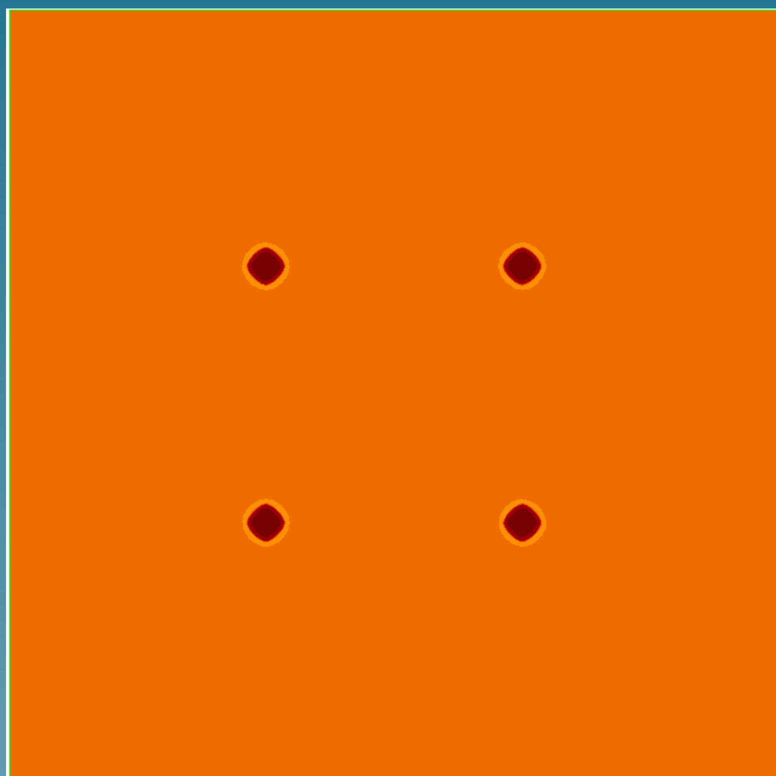
Results



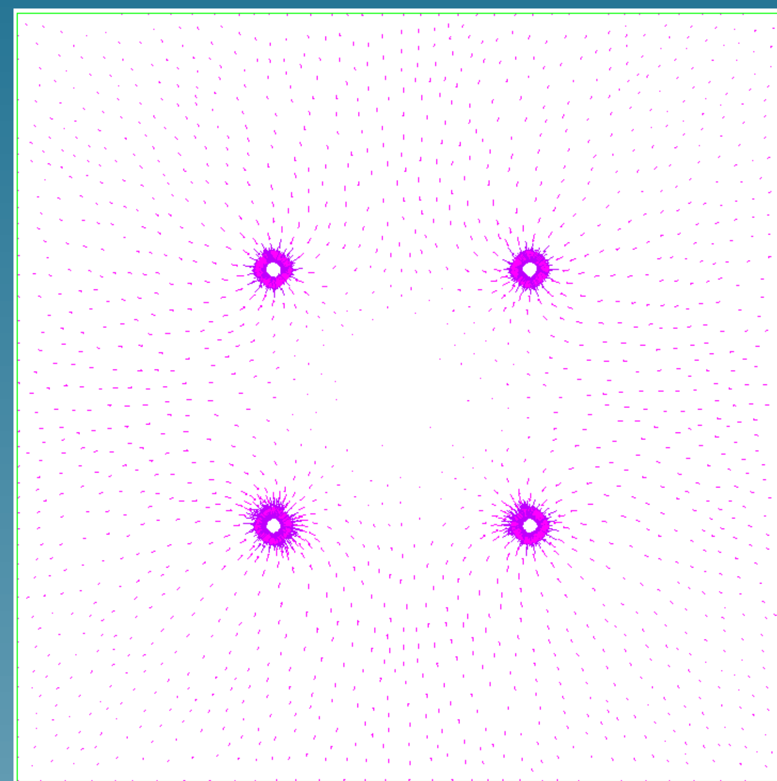
Conclusions and perspectives

- Dendritic growth and coalescence : adaptive finite elements with high aspect ratio $\longrightarrow$ accurate results with few vertices ($< 20\ 000$).
- Mathematical analysis of coalescence.
- Dendritic growth and coalescence with convection.
- 3D ?

Dendritic growth and coalescence with convection

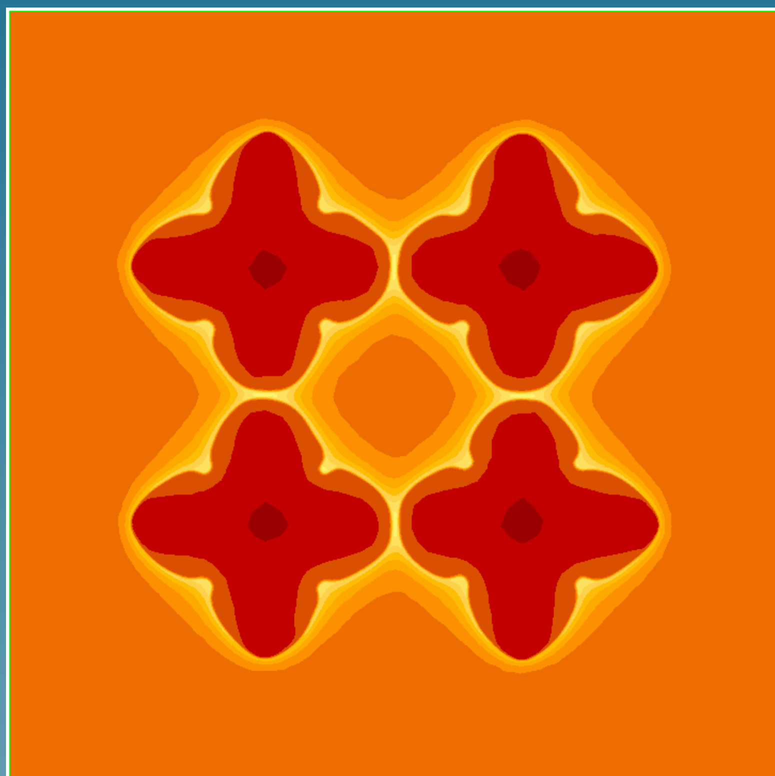


Concentration

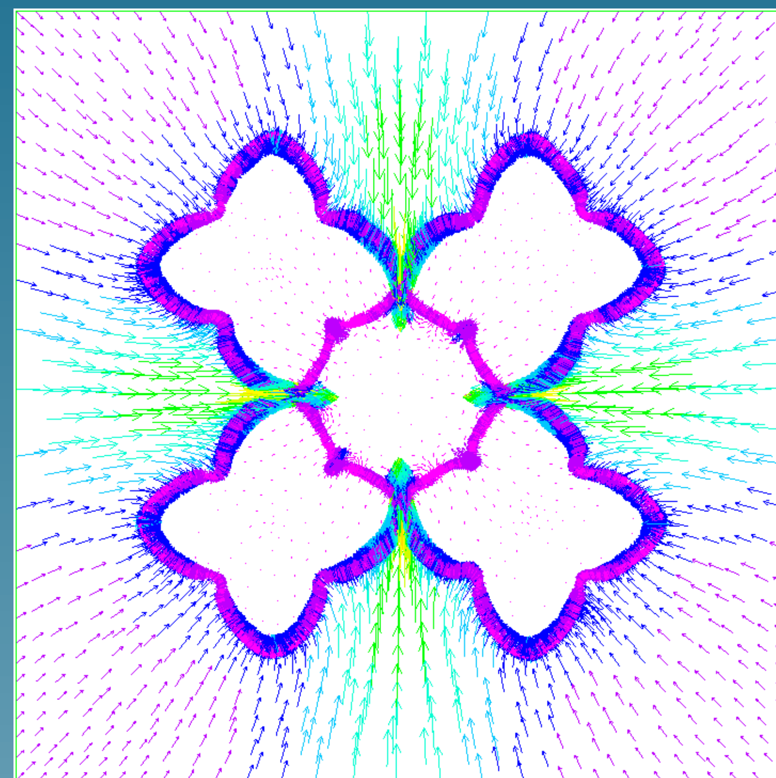


Velocity

Dendritic growth and coalescence with convection



Concentration



Velocity