3D adaptive finite elements with high aspect ratio for the computation of dendritic growth with convection

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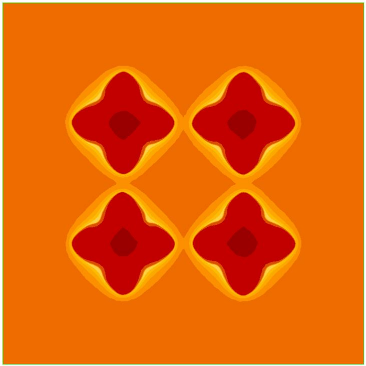
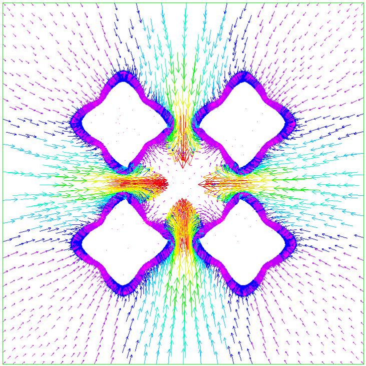
Outline

- Goal: take into account fluid flow between dendrites due to variable solid and liquid densities (shrinkage).
- Tool: adaptive finite elements with high aspect ratio.

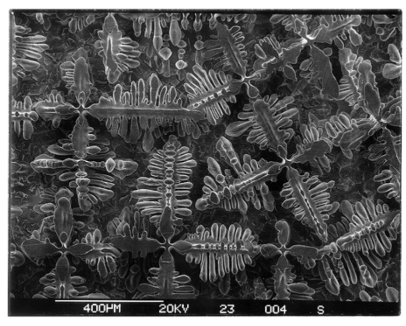


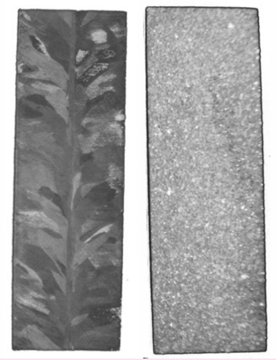
concentration



velocity

Solidification: Dendritic growth



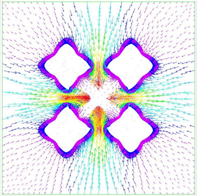


Lenght scales

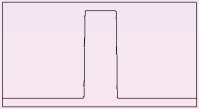
- Workpiece $\simeq 1\ m$
- Dendrite $\simeq 10^{-3}\ m$
- Solid-liquid interface $\simeq 10^{-8}\ m$ (100 atoms)

The unknowns

concentration



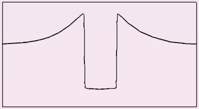
velocity



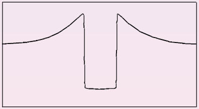
Phase field ϕ

$\phi = 0$: liquid

$\phi = 1$: solid



Concentration c



Velocity $\mathbf{u}$

Temperature $T(x, y, t)$ is a parameter

The model with convection

Governing equations

- Phase field:

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

- Concentration:

$$\frac{\partial c}{\partial t} + \operatorname{div}\Big(G(\phi,\mathbf{u},c)\Big) - \operatorname{div}\Big(D_1(\phi)\nabla c + D_2(c,\phi)\nabla\phi\Big) = 0$$

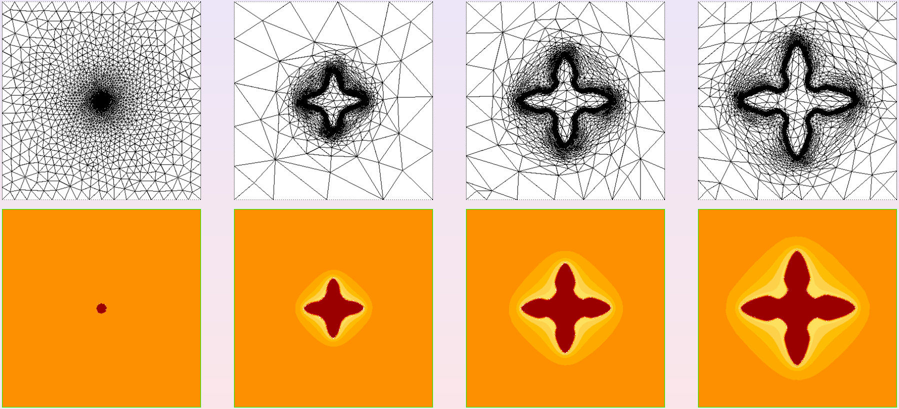
- Fluid flow:

$$\rho = \phi\rho_s + (1-\phi)\rho_l$$

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} - \mu\Delta\mathbf{u} + \nabla p + \operatorname{div}\Big(\mathbf{F}(\phi,\mathbf{u})\Big) + \frac{1}{\epsilon}\phi^2\mathbf{u} = 0$$

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho\mathbf{u}) = 0$$

Adaptive finite elements with large aspect ratio



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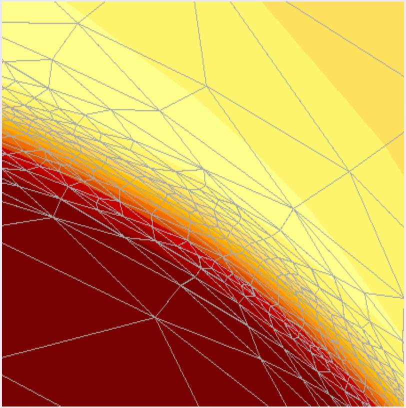
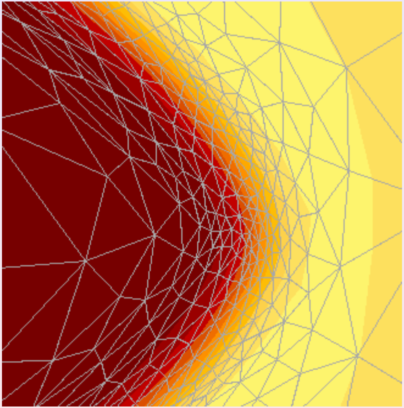




Same precision with isotropic meshes: 10 to 100 times more vertices!

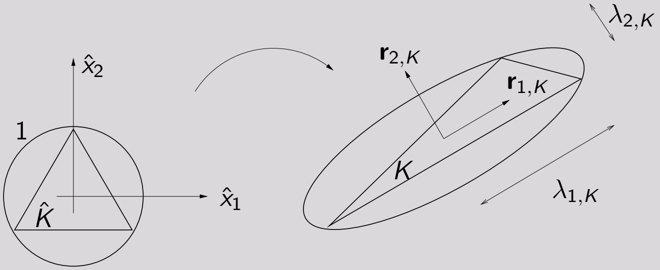
A posteriori error estimates

- Dendritic growth without convection

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

- Existence for low physical anisotropy, a priori error estimates (Burman Rappaz M3AS 2003).
- A posteriori error estimates, adaptive FE with high aspect ratio, numerical study of the effectivity index (Burman Picasso J. Interfaces Free Boundaries 2003).
- No theory with convection

Error estimator for meshes with high aspect ratio



$e = c - c_h,$

$$\eta_K^2 = \int_{t^{n-1}}^{t^n} \frac{1}{\sqrt{\lambda_{2,K}}} \left\| \left[\frac{\partial c_h}{\partial n} \right] \right\|_{L^2(\partial K)} \sqrt{\lambda_{1,K}^2 \left(\mathbf{r}_{1,K}^T G_K(e) \mathbf{r}_{1,K} \right) + \lambda_{2,K}^2 \left(\mathbf{r}_{2,K}^T G_K(e) \mathbf{r}_{2,K} \right)}$$

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$$G_K(e) = \begin{pmatrix} \int_K \left(\frac{\partial e}{\partial x_1} \right)^2 & \int_K \frac{\partial e}{\partial x_1} \frac{\partial e}{\partial x_2} \\ \int_K \frac{\partial e}{\partial x_1} \frac{\partial e}{\partial x_2} & \int_K \left(\frac{\partial e}{\partial x_2} \right)^2 \end{pmatrix}$$

Zienkiewicz-Zhu (ZZ) error estimator $\int_K \left(\frac{\partial e}{\partial x_1} \right)^2 \to \int_K \left(\frac{\partial u_h}{\partial x_1} - \Pi \frac{\partial u_h}{\partial x_1} \right)^2$

Error estimator equivalent to the true error for adapted meshes

$$C_1 \eta_K \leq \textit{true error} \leq C_2 \eta_K$$

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

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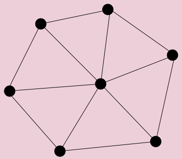

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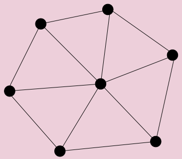

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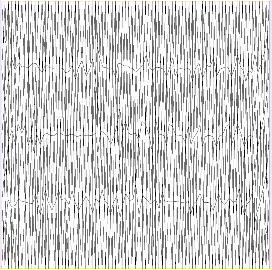
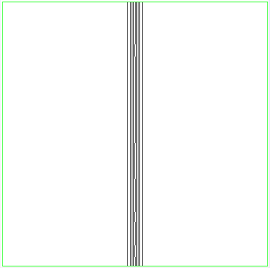
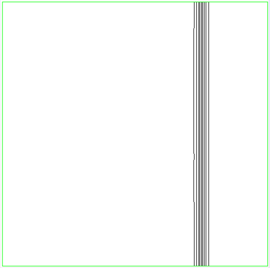
Numerical validation of the error indicator



mesh



ϕ, c at initial time



ϕ, c at final time

$h1 - h2$	error	ei
0.000005 – 0.0001	0.29	1.85
0.0000025 – 0.00005	0.13	1.74
0.00000125 – 0.000025	0.066	1.74

ei: effectivity index, error indicator / true error.

Adaptive algorithm

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

$$0.75\ TOL \leq \frac{\left(\sum_K \eta_K^2\right)^{1/2}}{\left(\int_\Omega |\nabla u_h|^2\right)^{1/2}} \leq 1.25\ TOL$$

Sufficient condition : $0.75^2\, TOL^2 \int_K |\nabla u_h|^2 \leq \eta_K^2 \leq 1.25^2\, TOL^2 \int_K |\nabla u_h|^2$

Equidistribute the error in directions 1 and 2

Align the triangle with the eigenvectors of $G_K(e)$

Use the BL2D mesh generator (INRIA)
(Meshadapt software (INRIA) in 3D)

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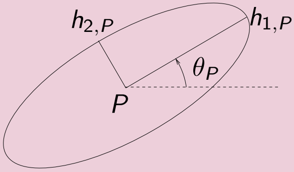

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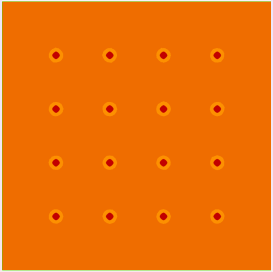
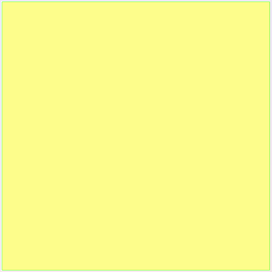
Numerical results in 2D : 16 dendrites

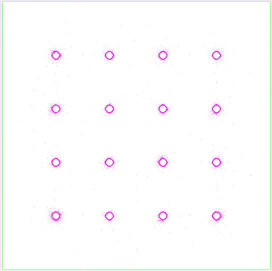
Time 0.025 s



concentration



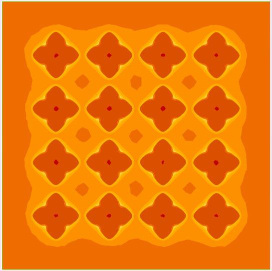
pressure



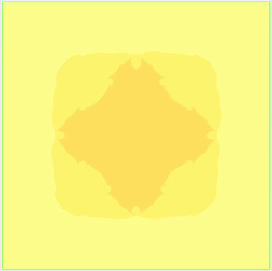
velocity

Numerical results in 2D : 16 dendrites

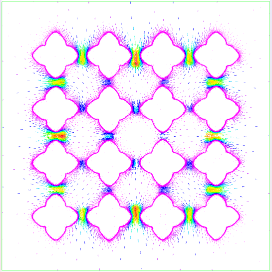
Time 0.15 s



concentration



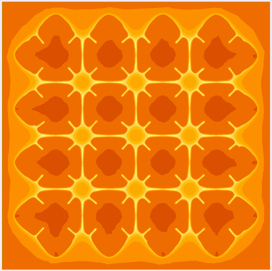
pressure

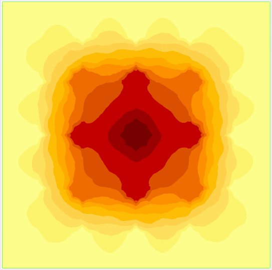


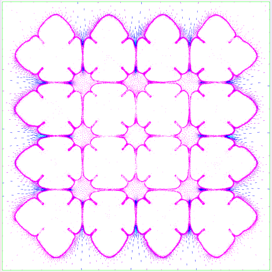
velocity

Numerical results in 2D : 16 dendrites

Time 0.225 s


concentration


pressure


velocity

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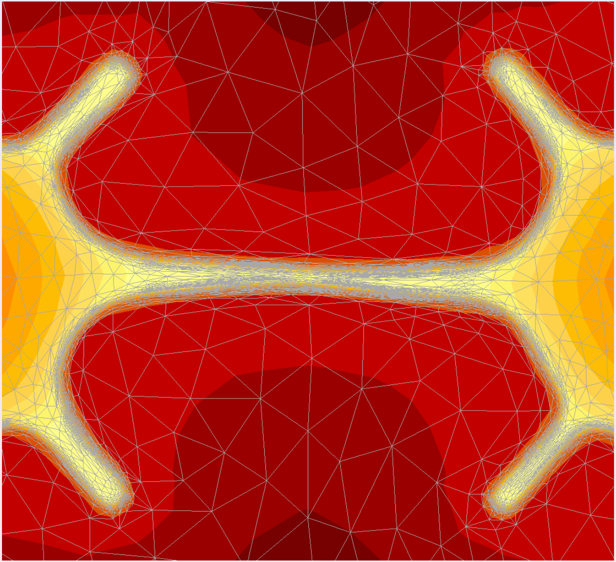
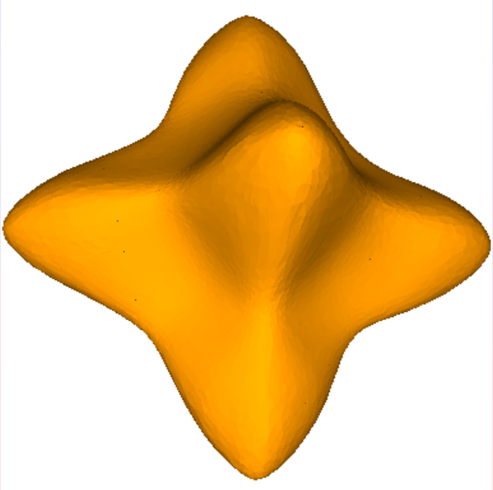
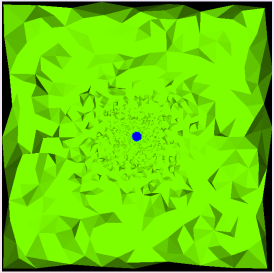


Numerical results in 3D : 1 dendrite

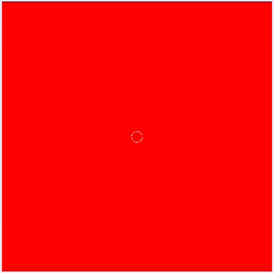


Numerical results in 3D : 1 dendrite

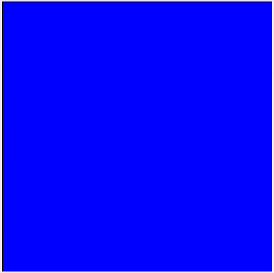
Time 0.25 s



concentration



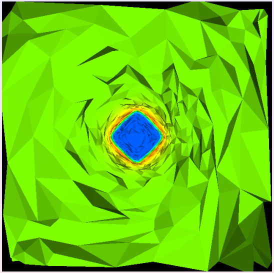
pressure



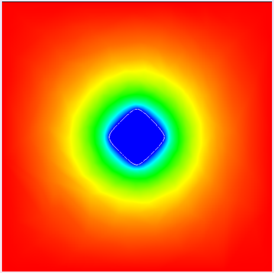
velocity

Numerical results in 3D : 1 dendrite

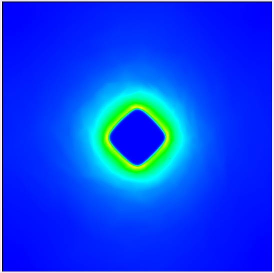
Time $0.50\ s$



concentration



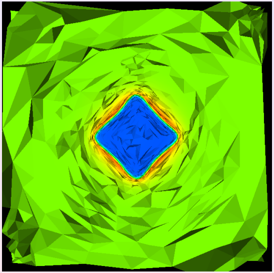
pressure



velocity

Numerical results in 3D : 1 dendrite

Time 0.50 s



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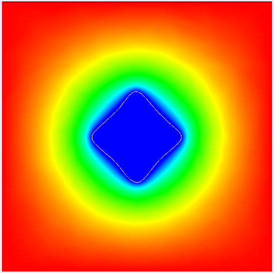

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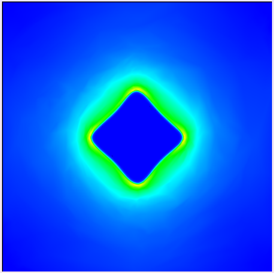

velocity

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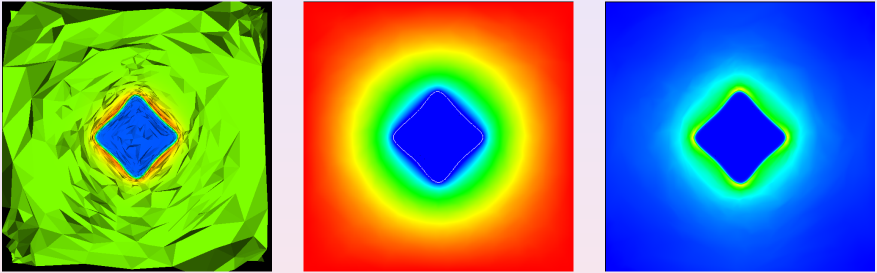
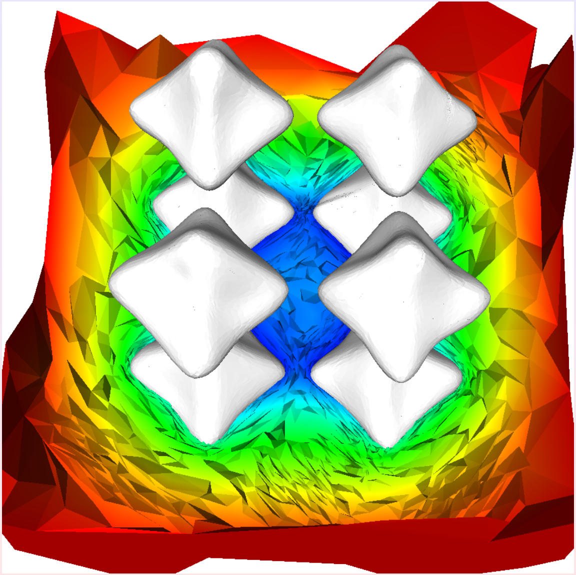


concentration pressure velocity

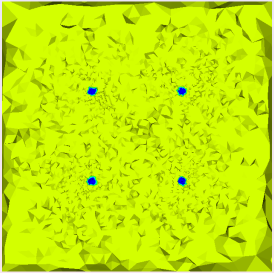
Maximal number of vertices : 138487
Average aspect ratio : 77.68

Numerical results in 3D : 8 dendrites



Numerical results in 3D : 8 dendrites

Time 0.00 s



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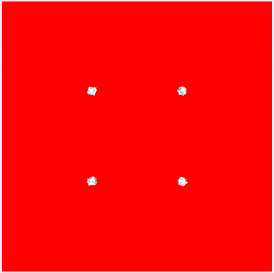
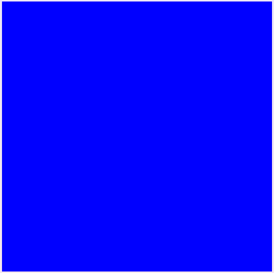


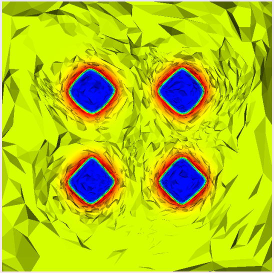
pressure



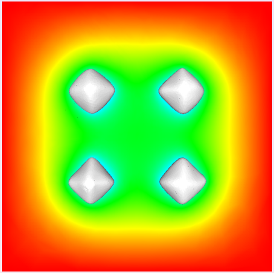
velocity

Numerical results in 3D : 8 dendrites

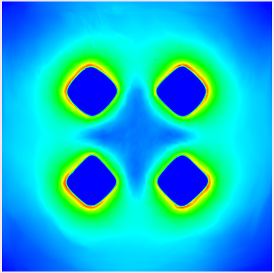
Time 0.25 s



concentration



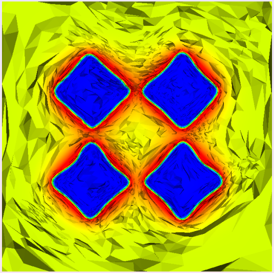
pressure



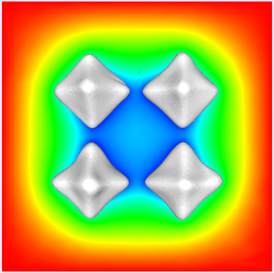
velocity

Numerical results in 3D : 8 dendrites

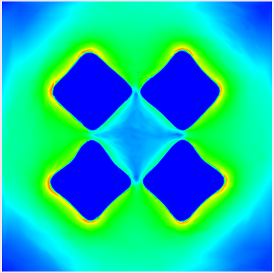
Time 0.50 *s*



concentration



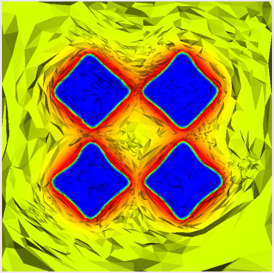
pressure



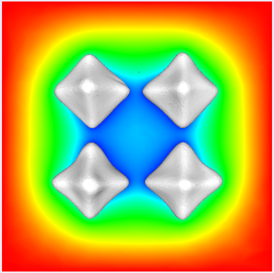
velocity

Numerical results in 3D : 8 dendrites

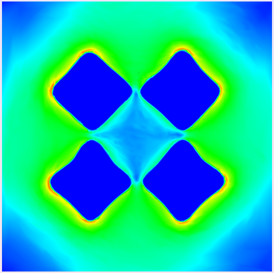
Time 0.50 s



concentration



pressure



velocity

Maximal number of vertices : 256263
Average aspect ratio : 11.51

Conclusions and perspectives

- Anisotropic, adaptive meshes make 3D simulations possible on a single PC.
- Theoretical justification ? Use of several error estimators ?
- Micro - macro coupling ?