Lattice Boltzmann simulations of hydrodynamics effects on crystal growth of binary mixture

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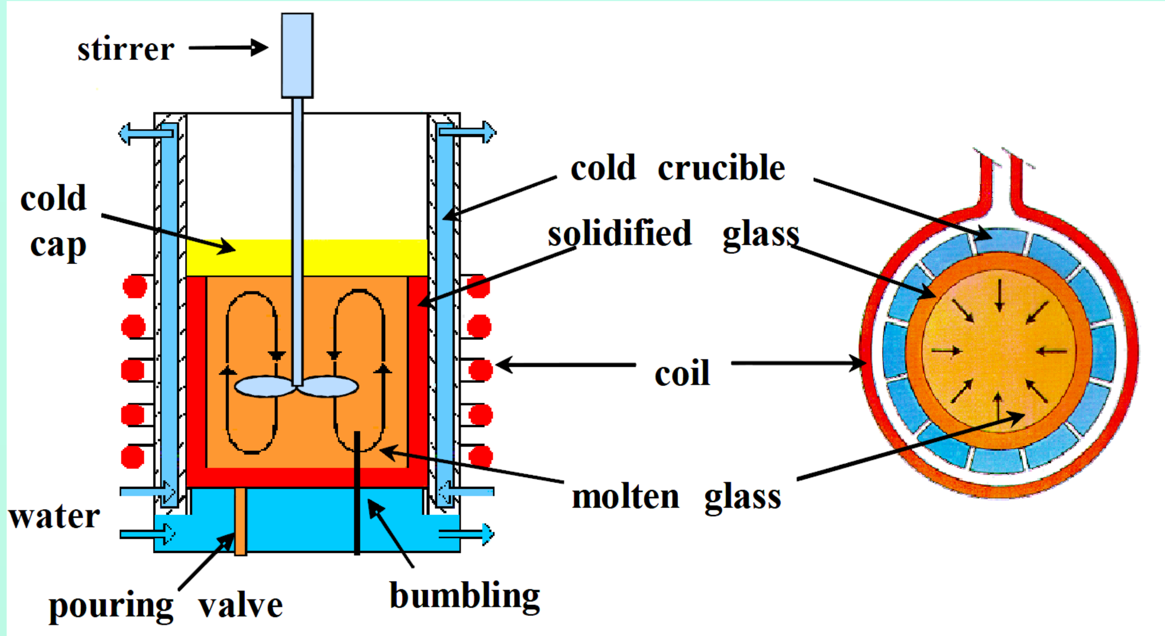
Context

Principle of vitrification by cold crucible

- ✓Partial crystallization of glass involved in cold crucible (crystallization of skull melter).
- ✓Simulation method for vitrification by the technique of cold crucible.



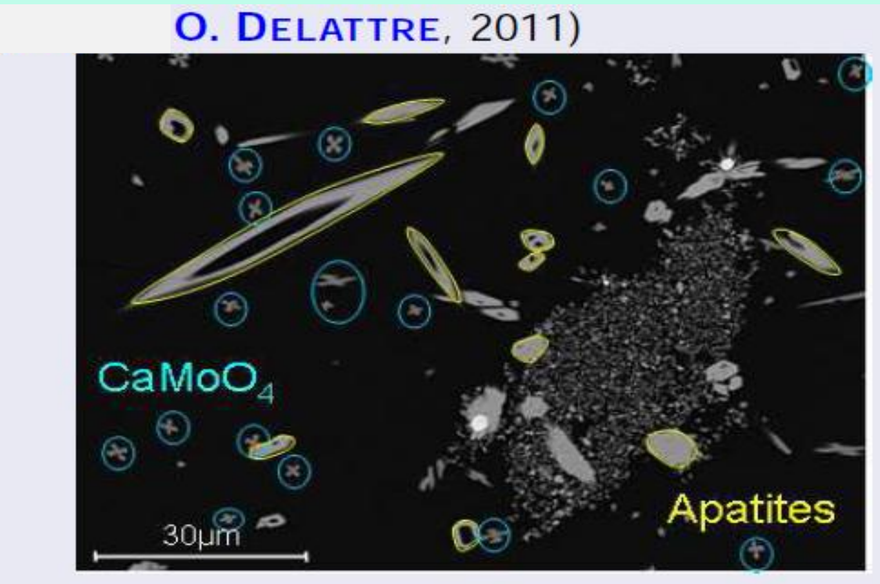
Objective

- ✓ Dynamics of crystal growth and morphology modeling
- ✓Solidification of a binary mixture.

Experiments and observations carried out by E. Régnier and S. Schuller

Observation of crystallization in the glass

O. Delattre, 2011)



Mathematical model (binary mixture)

Phase-Field Model

$$\tau(\mathbf{n})\frac{\partial\phi}{\partial t} = W_0^2\nabla\cdot(a_s^2(\mathbf{n})\nabla\phi) + W_0^2\sum_{\alpha=x,y,z}\frac{\partial}{\partial\alpha}\left(|\nabla\phi|^2 a_s(\mathbf{n})\frac{\partial a_s(\mathbf{n})}{\partial(\partial_\alpha\phi)}\right) + (\phi-\phi^3) - \lambda(Mc_\infty U+\theta)(1-\phi^2)^2$$

$$\left(\frac{1+k}{2}-\frac{1-k}{2}\phi\right)\frac{\partial U}{\partial t} + \left(\frac{1-\phi}{2}\right)\mathbf{V}\cdot\nabla U = \nabla\cdot(Dq(\phi)\nabla U - \mathbf{J}_{at}) + [1+(1-k)U]\frac{1}{2}\frac{\partial\phi}{\partial t}$$

$$\frac{\partial\theta}{\partial t} + \left(\frac{1-\phi}{2}\right)\mathbf{V}\cdot\nabla\theta = \kappa\nabla^2\theta + \frac{1}{2}\frac{\partial\phi}{\partial t}$$

Anisotropic function :

$$a_s(\mathbf{n}) = 1+\varepsilon_s\Big(\underbrace{\sum_{\alpha=x,y,z} n_\alpha^4}_{Q} - \frac{3}{5}\Big) + \delta\left(3Q + 66 n_x^2 n_y^2 n_z^2 - \frac{17}{7}\right)$$

Work in progress :

1. Extension of the model with two different specific heat in the two phases.
2. Coupling with flow: development of the model to include a density change between solid and liquid.

Numerical method

Collision and Streaming steps

$$f_i(\mathbf{x}+\mathbf{e}_i\delta x, t+\delta t) = f_i(\mathbf{x},t) - \frac{1}{\zeta_U}\left(f_i(\mathbf{x},t) - f_i^{(0)}(\mathbf{x},t)\right) + w_i\left[E(\mathbf{x},t)+\frac{Q(\mathbf{x},t)}{\eta(\phi)}\right]$$

Equilibrium distribution functions

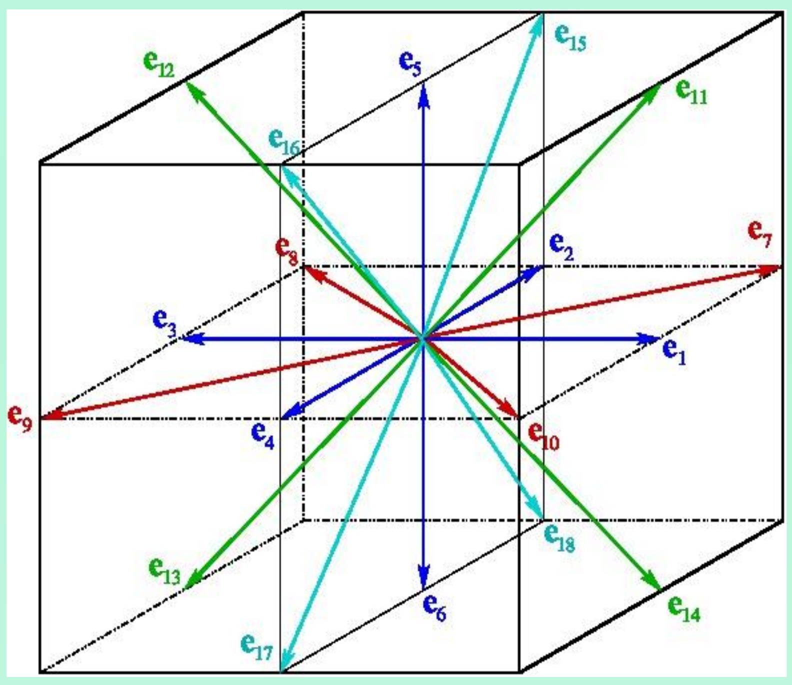
$$f_i^{(0)}(\mathbf{x},t) = A_i U(\mathbf{x},t) + B_i\left(\frac{Dq(\phi)}{\eta(\phi)}U(\mathbf{x},t) + \frac{1}{e^2}\mathbf{e}_i\cdot\mathbf{J}_{tot}\frac{\delta t}{\delta \mathbf{x}}\right)$$

$$\mathbf{J}_{tot}(\mathbf{x},t) = \left[\nabla\left(\frac{Dq(\phi)}{\eta(\phi)}\right) + Dq(\phi)\nabla\left(\frac{1}{\eta(\phi)}\right)\right]U(\mathbf{x},t) + \frac{\mathbf{J}_{at}(\mathbf{x},t)}{\eta(\phi)}$$

Update Boundary Conditions

Moment of order 0

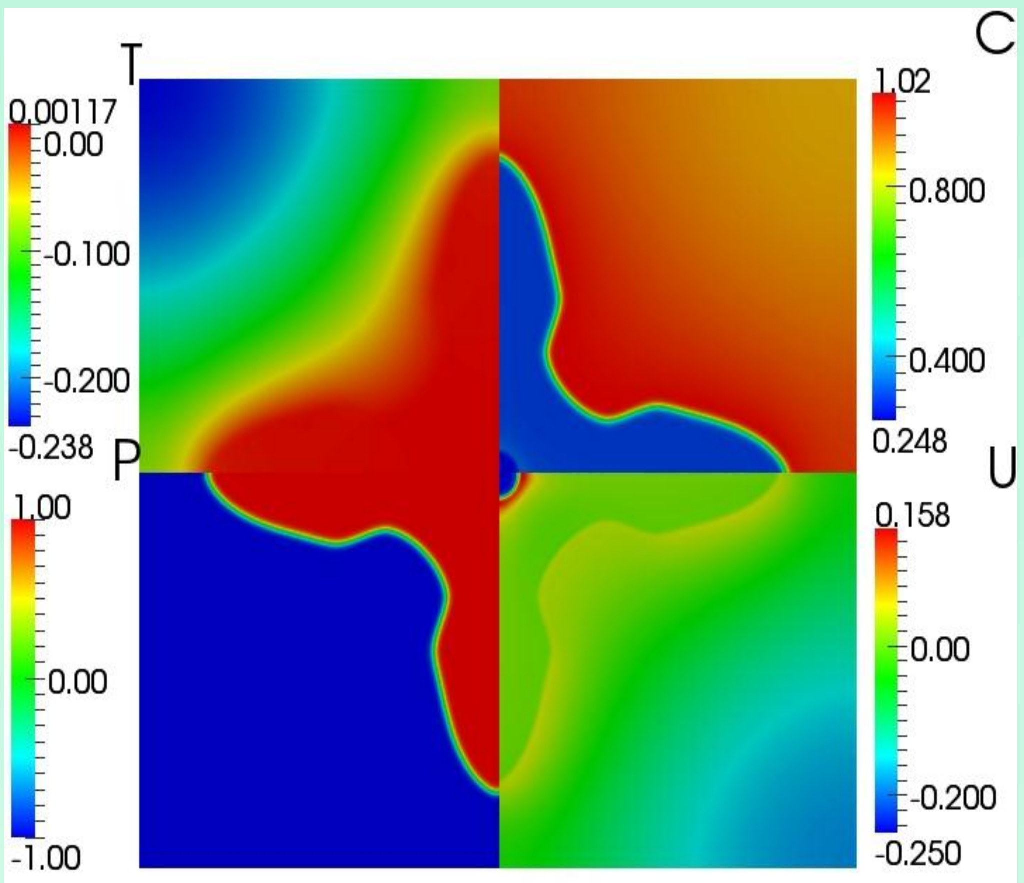
$$U(\mathbf{x},t)=\sum_{i=0}^{N} f_i(\mathbf{x},t)$$

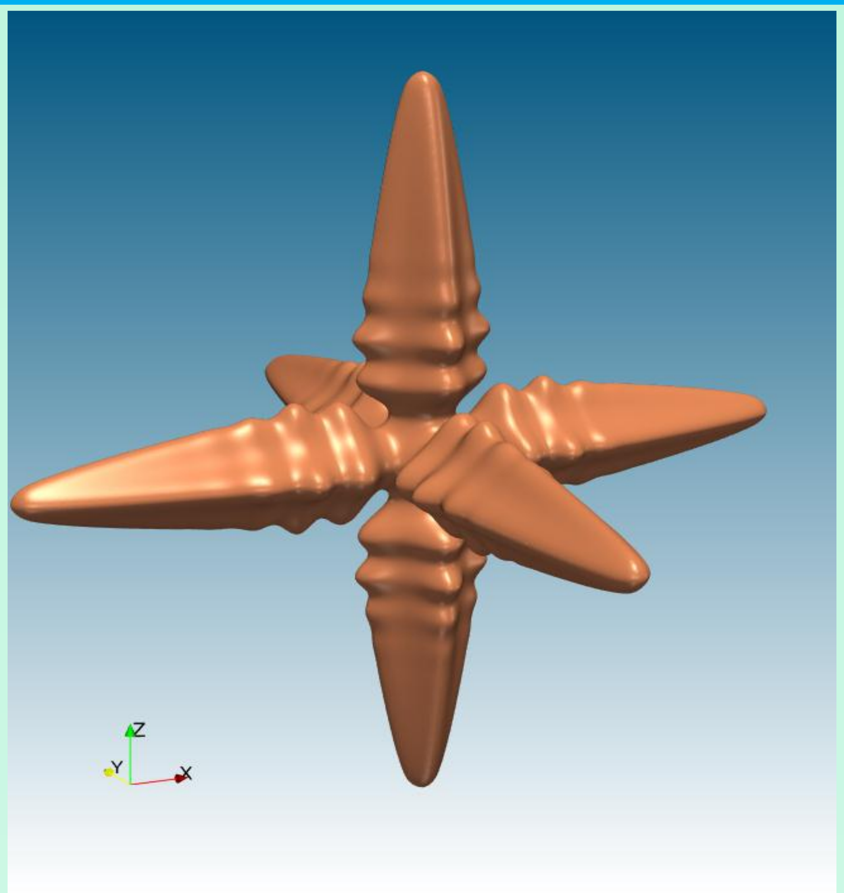


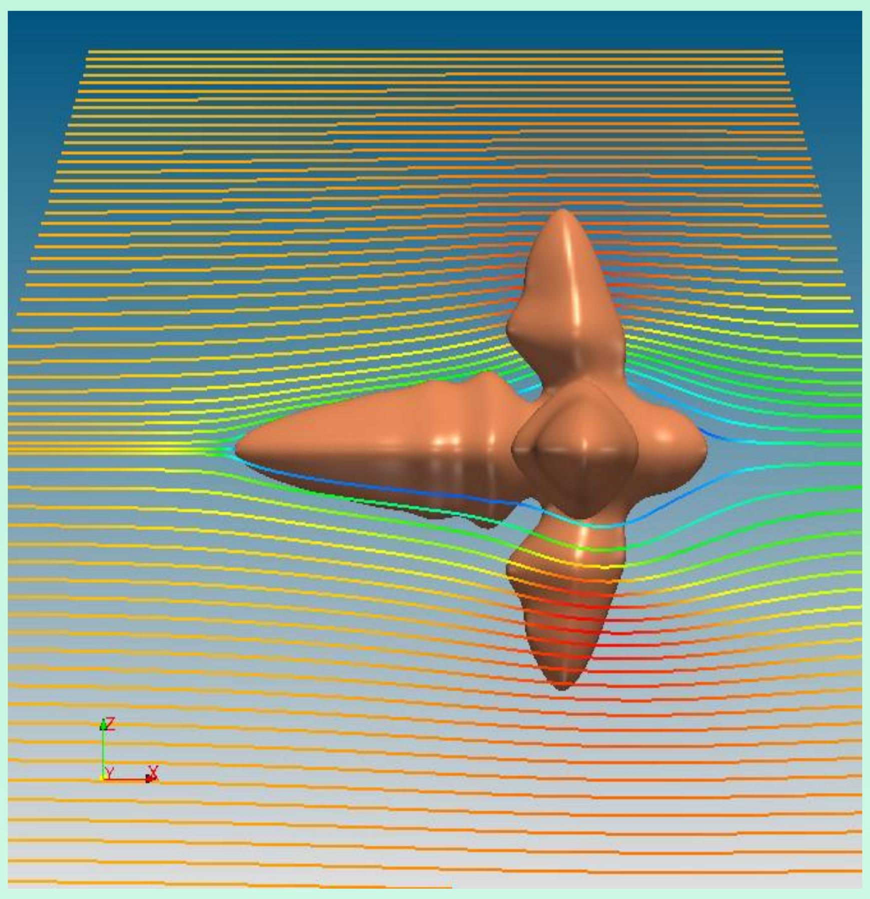
Phase field model [1] solved by using a Lattice Boltzmann method. The scheme is based on BGK approximations.

Details of numerical method are given in [2].

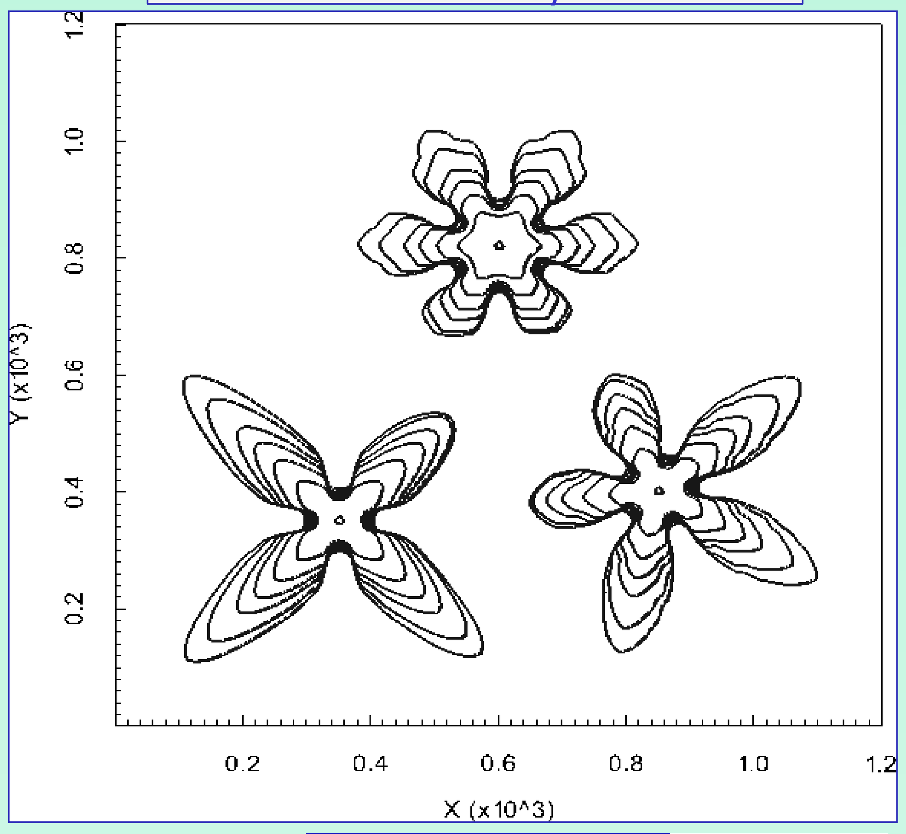
Numerical results

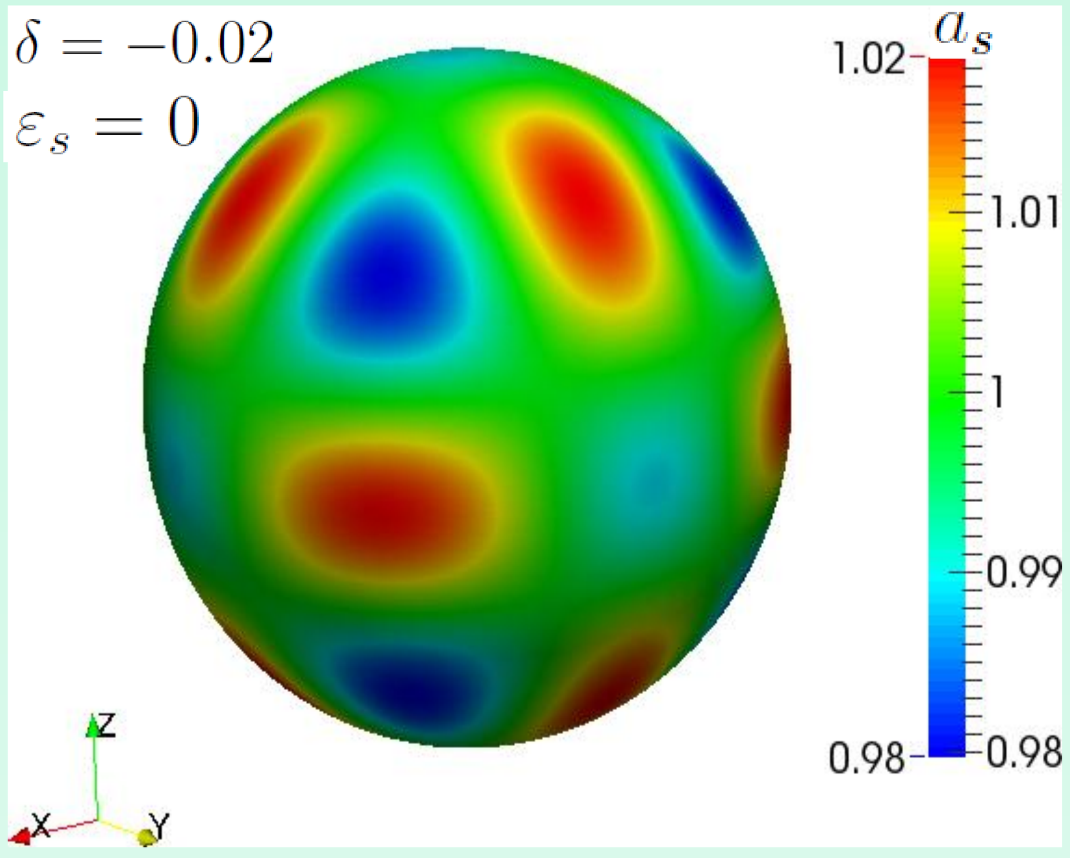


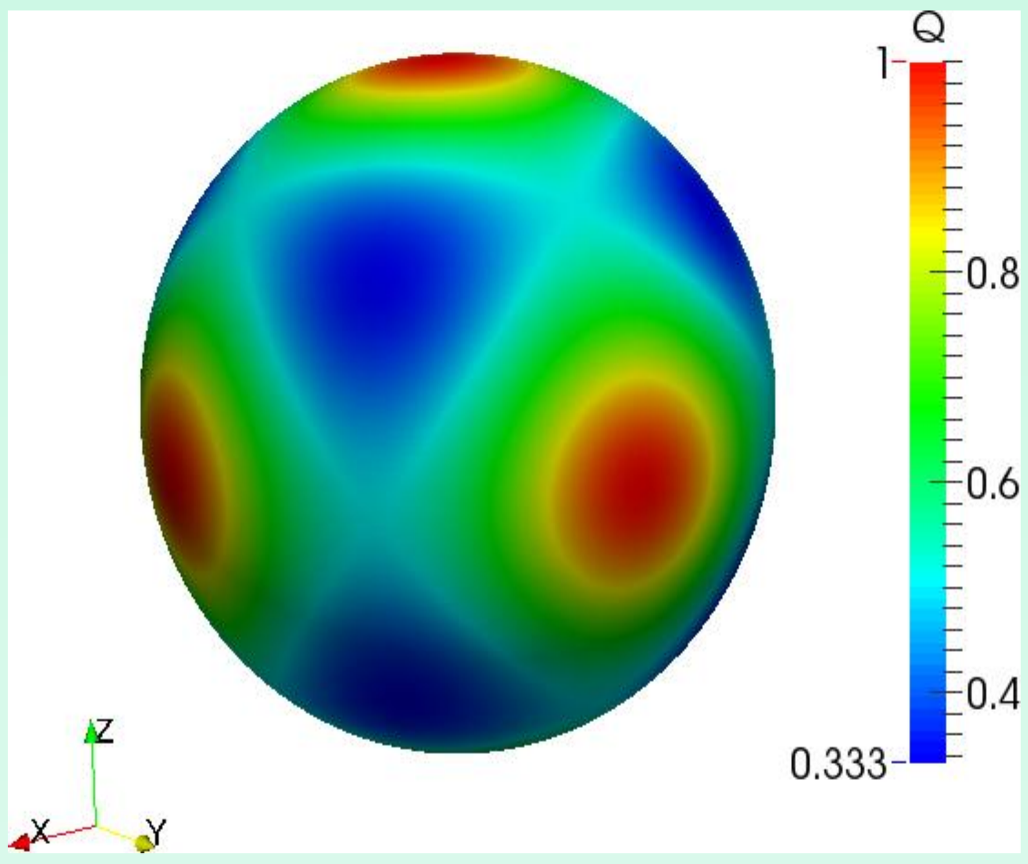


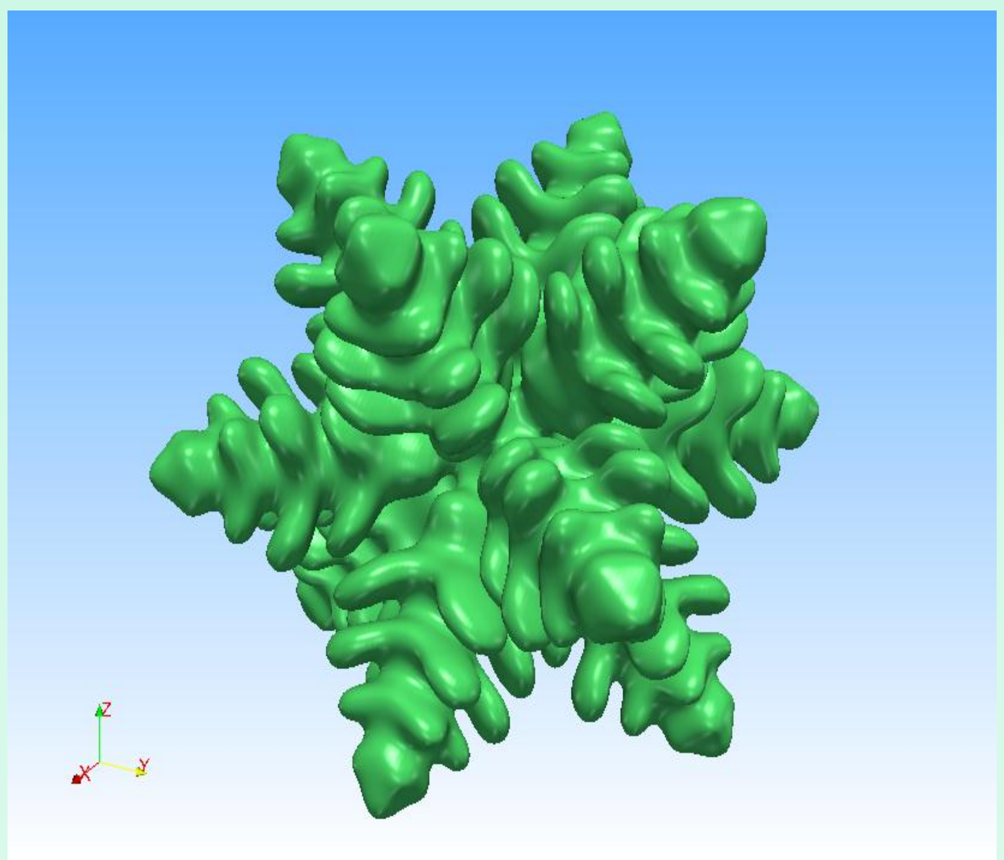


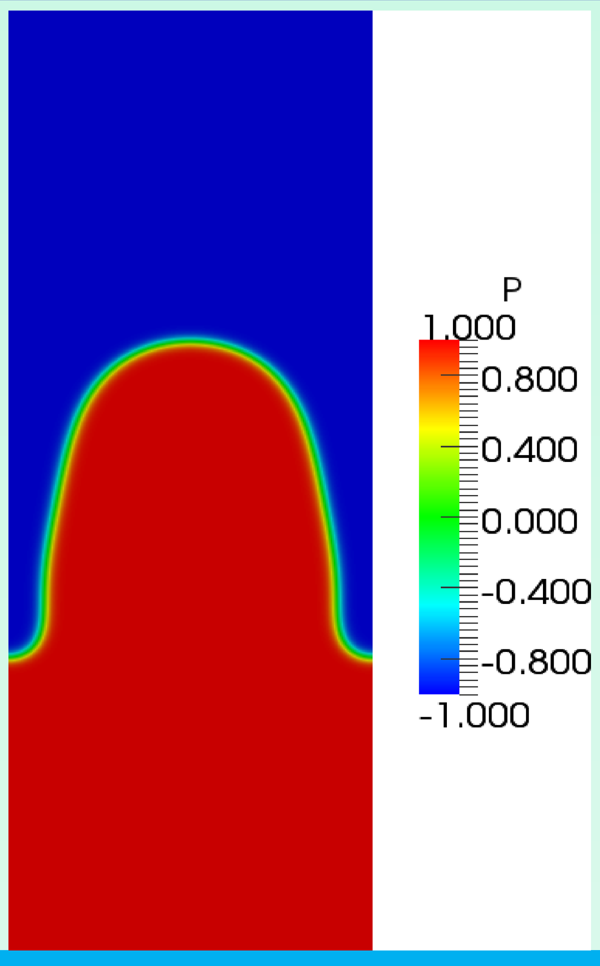
V. Hellaudais, 2014











References

[1] C. Ramirez, C. Beckermann, A. Karma, H.-J. Diepers, Physical Review E 69 (051607) (2004) 1–16.

[2] A. Younsi, A. Cartalade, M. Quintard, Proceeding IHTC-15 (2014). And other references.