
Phase-field simulations of solidification structures

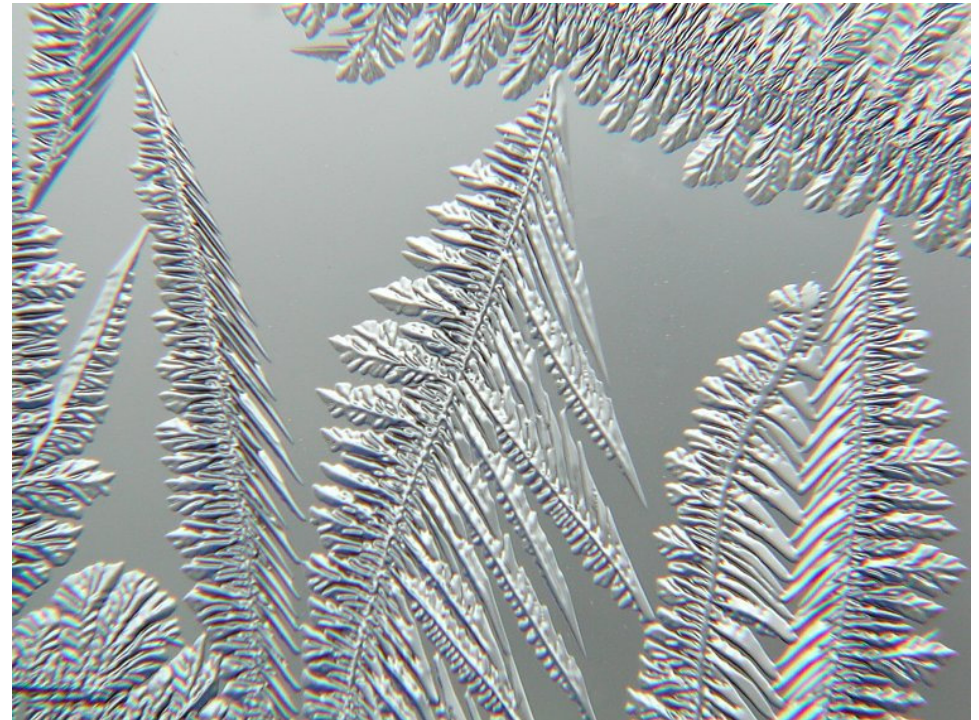
Denis Danilov

HS Karlsruhe



Introduction: Real Structures

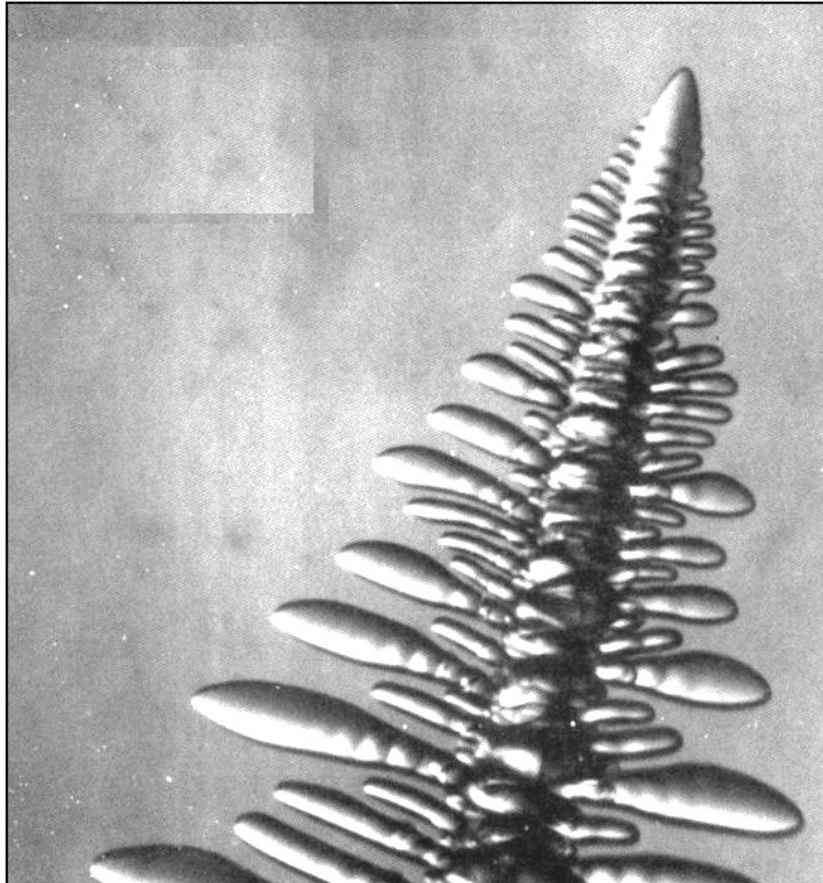
Experimental solidification structures: Snowflakes and Frost



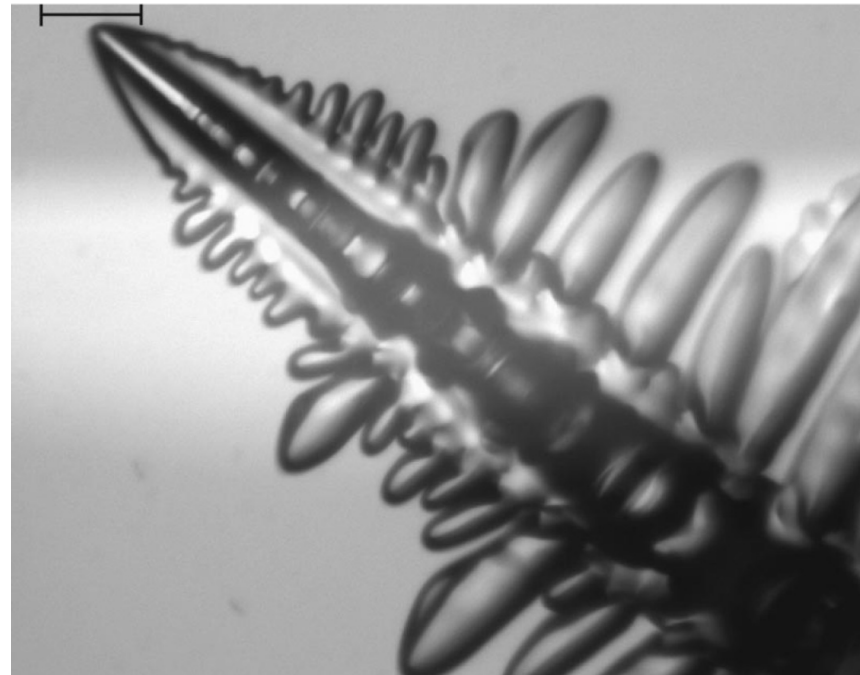
<http://www.its.caltech.edu/~atomic/snowcrystals/>

Real Structures

Experimental solidification structures: Dendrites in transparent materials

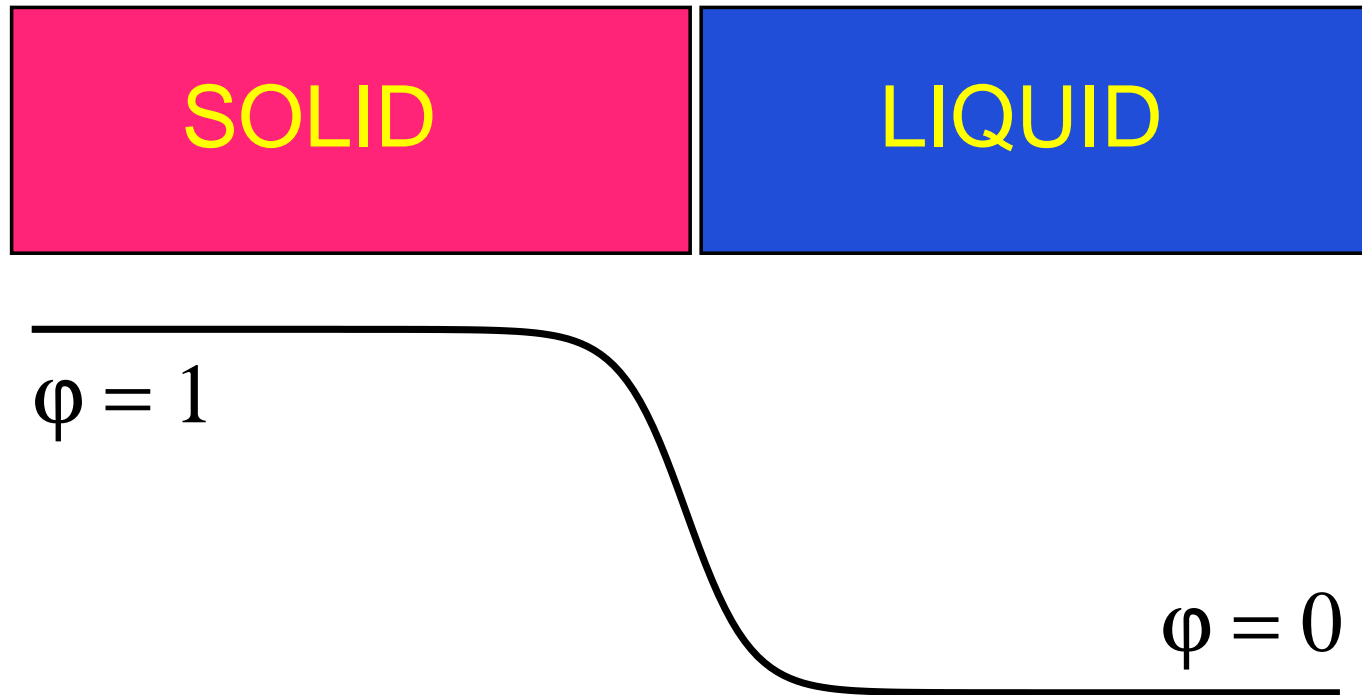


M. E. Glicksman
organic material



J. H. Bilgram, ETH Zürich
Xenon

Diffuse solid-liquid interface



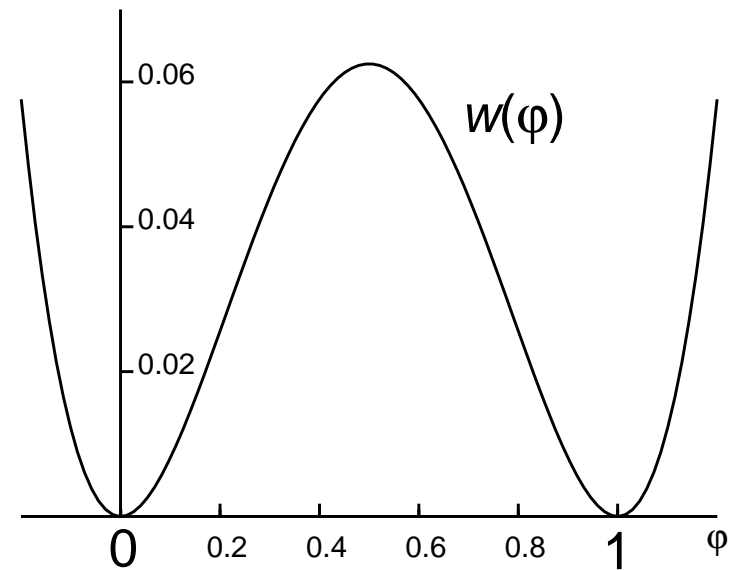
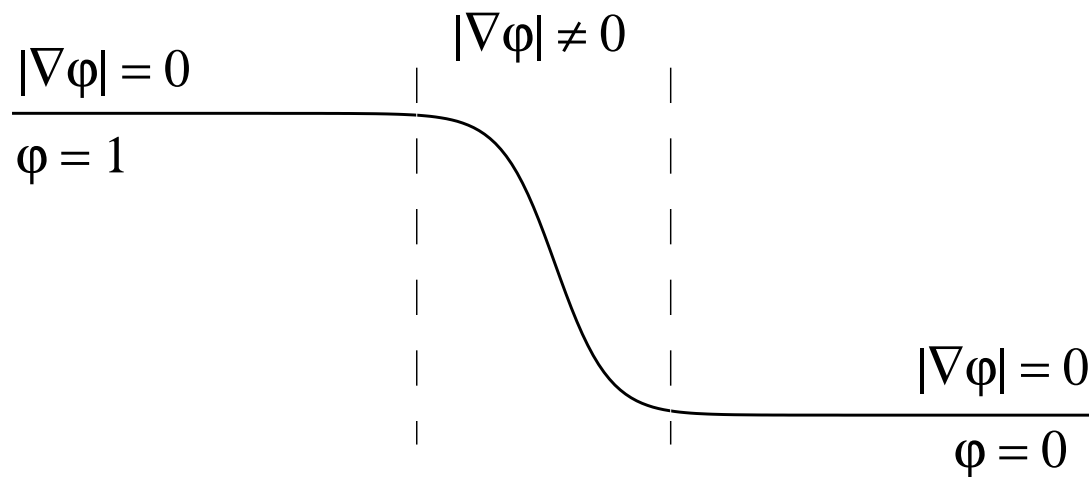
interface thickness (MD) $\sim 10\text{\AA}$

W. J. Boettinger, J. A. Warren, C. Beckermann, and A. Karma. Annu. Rev. Mater. Res. 32 (2002) 163

Phase-field model

– entropy functional

$$S(e, c, \varphi) = \int \left[s(e, c, \varphi) - \left(\varepsilon a(\nabla \varphi) + \frac{1}{\varepsilon} w(\varphi) \right) \right] dx,$$



$$a(\nabla \varphi) = \gamma(\nabla \varphi)^2, \quad w(\varphi) = 9\gamma g(\varphi), \quad g(\varphi) = \varphi^2(1 - \varphi)^2.$$

Phase-Field Model

– evolution of phase field

$$\partial_t \varphi \sim \frac{\delta S}{\delta \varphi},$$

$$2\omega\varepsilon\partial_t\varphi = 2\varepsilon\gamma\nabla^2\varphi - \frac{9\gamma}{\varepsilon}g_{,\varphi}(\varphi) - \frac{1}{T}f_{,\varphi}(c, \varphi),$$

phase-field parameters: $\varepsilon, \gamma, \omega$.

– free energy density ($T = \text{const}$)

$$f(c, \varphi) = \sum_{i=1}^2 c_i L_i \frac{T - T_i}{T_i} h(\varphi) + \frac{RT}{v_m} \sum_{i=1}^2 c_i \ln c_i,$$

$$h(\varphi) = \varphi^2(3 - 2\varphi).$$

Phase-Field Model

– chemical potential

$$\mu_i = f_{,c_i} = L_i \frac{T - T_i}{T_i} h(\varphi) + \frac{RT}{v_m} (\ln c_i + 1),$$

– mass fluxes

$$J_i = \sum_{j=1}^2 L_{ij} \nabla \frac{-\mu_j}{T},$$

$$L_{ij}(c, \varphi) = \frac{v_m}{R} D_i c_i \left(\delta_{ij} - \frac{D_j c_j}{\sum_{k=1}^2 D_k c_k} \right),$$

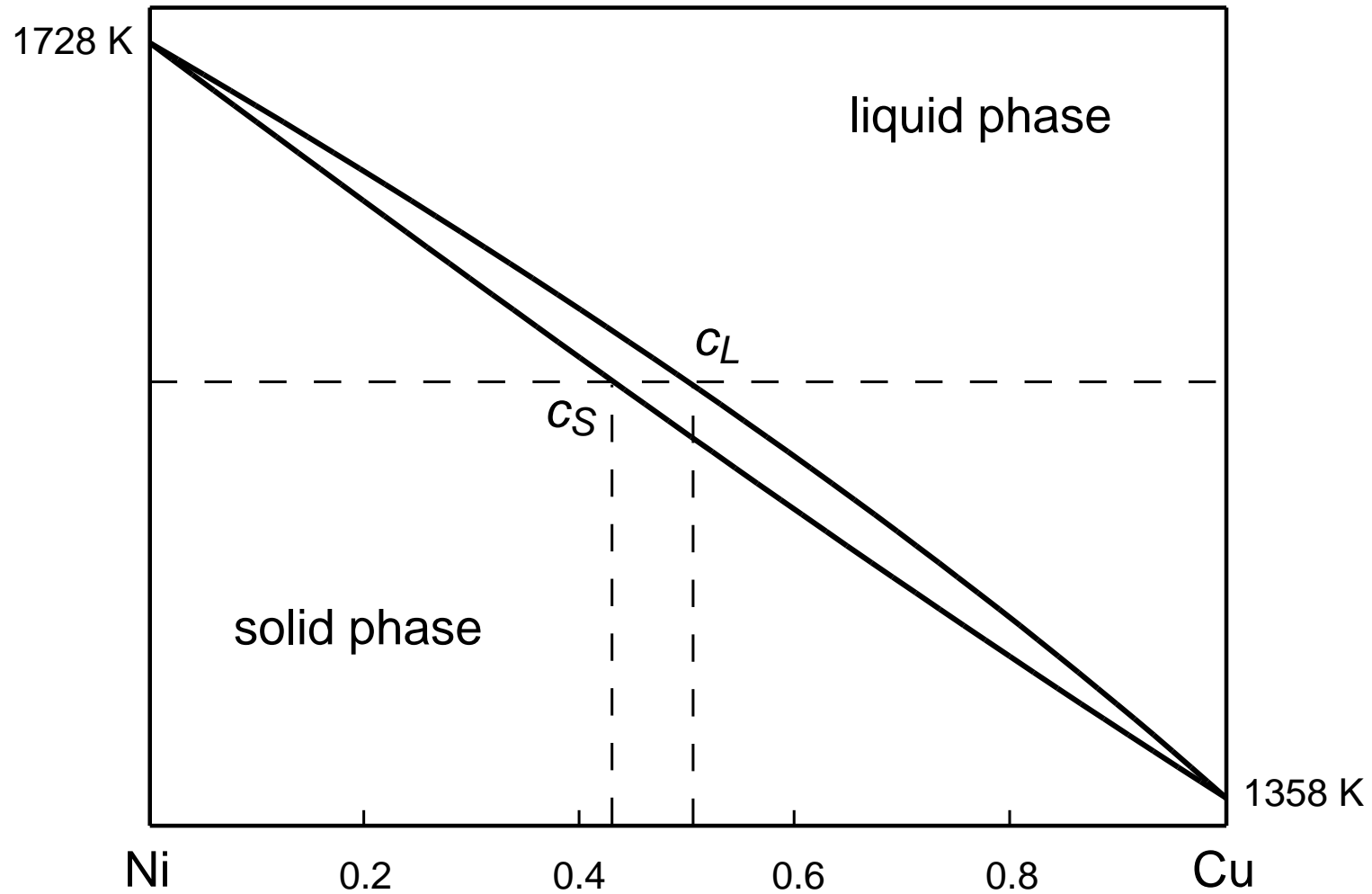
$$c_1 + c_2 = 1.$$

H. Garcke, B. Nestler, B. Stinner, *A diffuse interface model for alloys with multiple components and phases*, SIAM J. Appl. Math. **64**(3) (2004) 775–799.



Binary alloy

Equilibrium phase diagram



Binary alloy: Evolution equations

– phase field (nonconserved field)

$$\frac{\partial \varphi}{\partial t} = \frac{\varepsilon^2}{L^2} \nabla^2 \varphi - \frac{9}{2} \frac{dg}{d\varphi} - \frac{\varepsilon}{2\gamma} \Lambda(c, u) \frac{dh}{d\varphi}$$

$$\Lambda(c, u) = (1 - c_0 c) \frac{L_A}{T_A} \frac{u + (T_0 - T_A)/T_Q}{u + T_0/T_Q} + c_0 c \frac{L_B}{T_B} \frac{u + (T_0 - T_B)/T_Q}{u + T_0/T_Q}$$

– concentration field (conserved field)

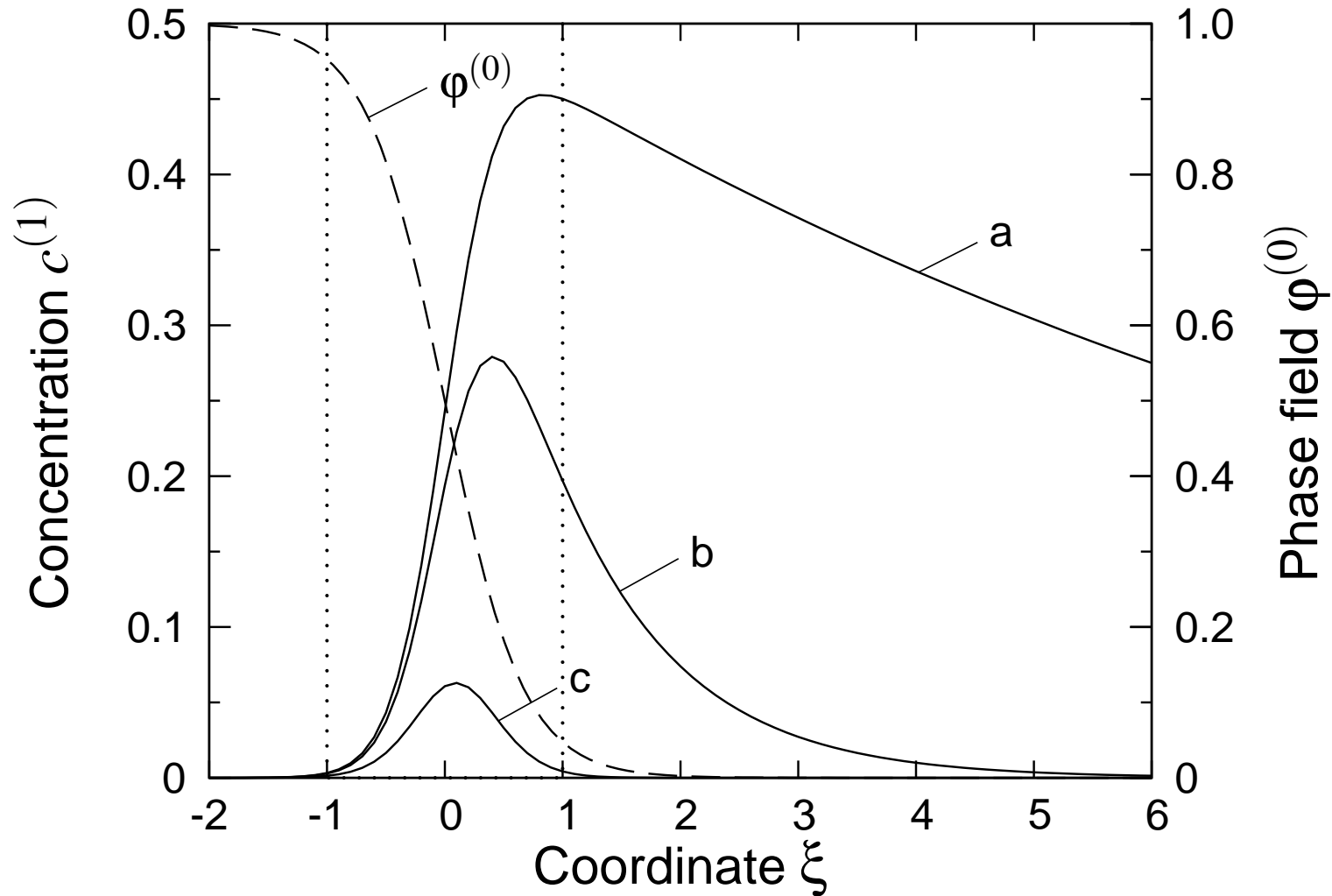
$$\frac{\partial c}{\partial t} = \nabla(\bar{D} \nabla c) - \nabla(\bar{D} c (1 - c_0 c) \nabla(\Theta(u) h(\varphi)))$$

$$\bar{D} = \frac{D}{\nu} \frac{\varepsilon^2}{L^2}$$

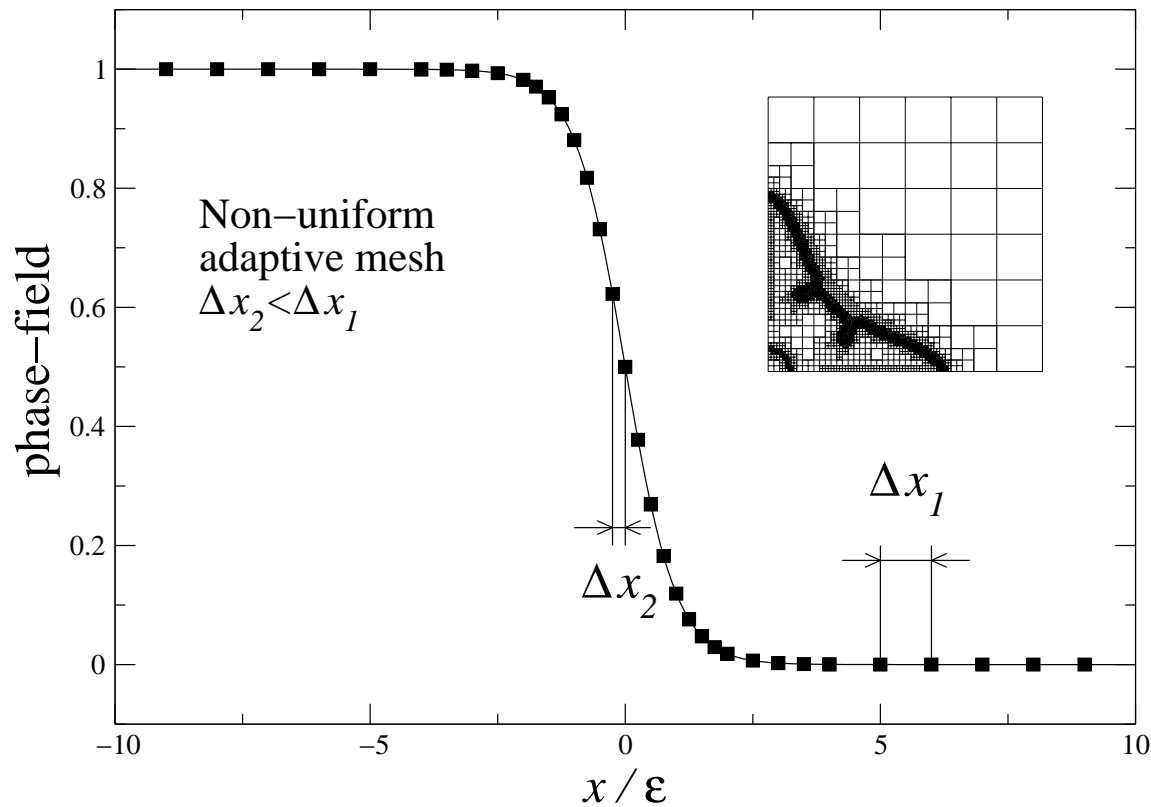
$$\Theta(u) = \frac{v_m}{R} \left(\frac{L_A}{T_A} \frac{u + (T_0 - T_A)/T_Q}{u + T_0/T_Q} - \frac{L_B}{T_B} \frac{u + (T_0 - T_B)/T_Q}{u + T_0/T_Q} \right)$$

Different length scales

Concentration profiles at different growth velocities



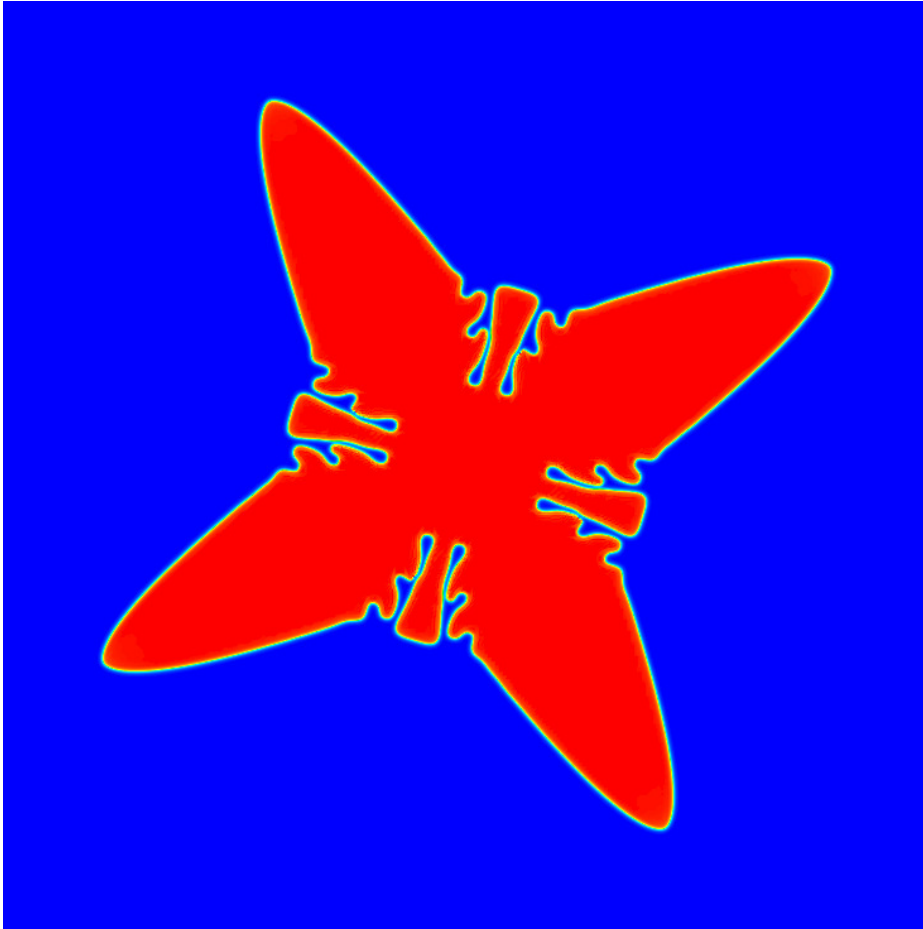
Adaptive grid spacing



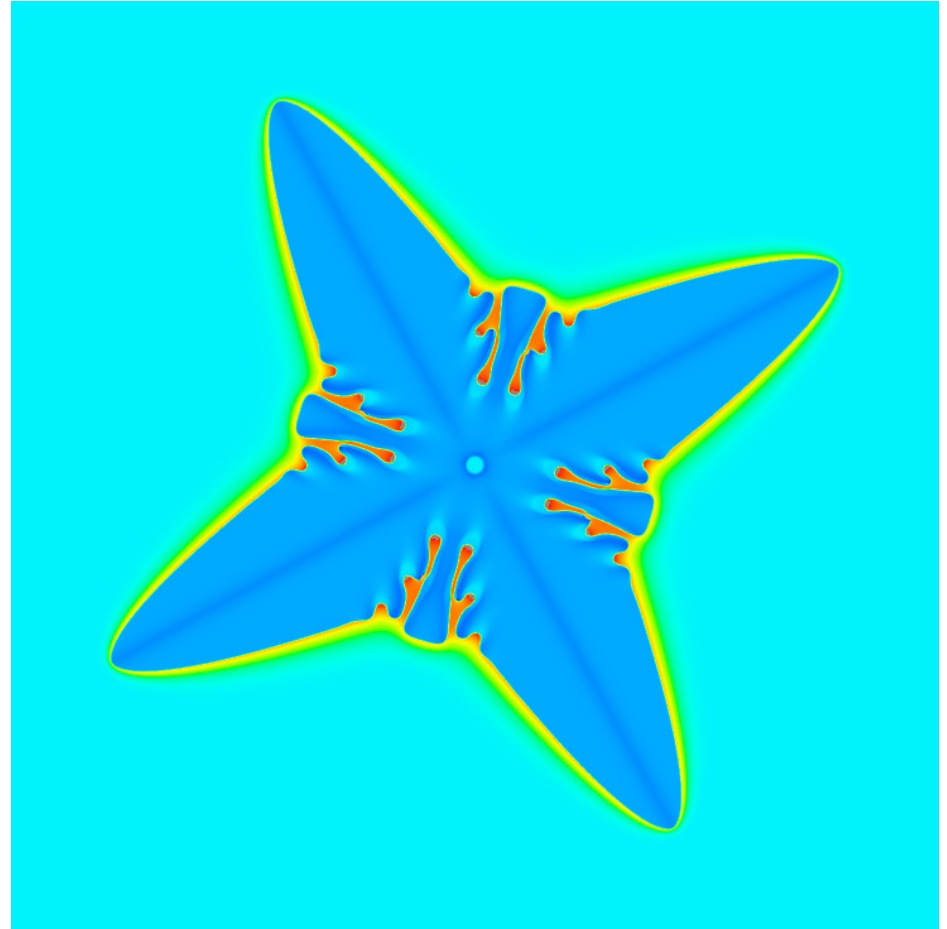
$$E = \sum_{\alpha} |\nabla \phi_{\alpha}| d^2 + E_C \sum_j |\nabla c_j| d^2 + E_T |\nabla T| d^2.$$

The cell will be refined if $E > E_{max}$ and coarsened if $E < E_{min}$. By this choice, $d \sim 1/\sqrt{E}$.

FEM: phase field and concentration field

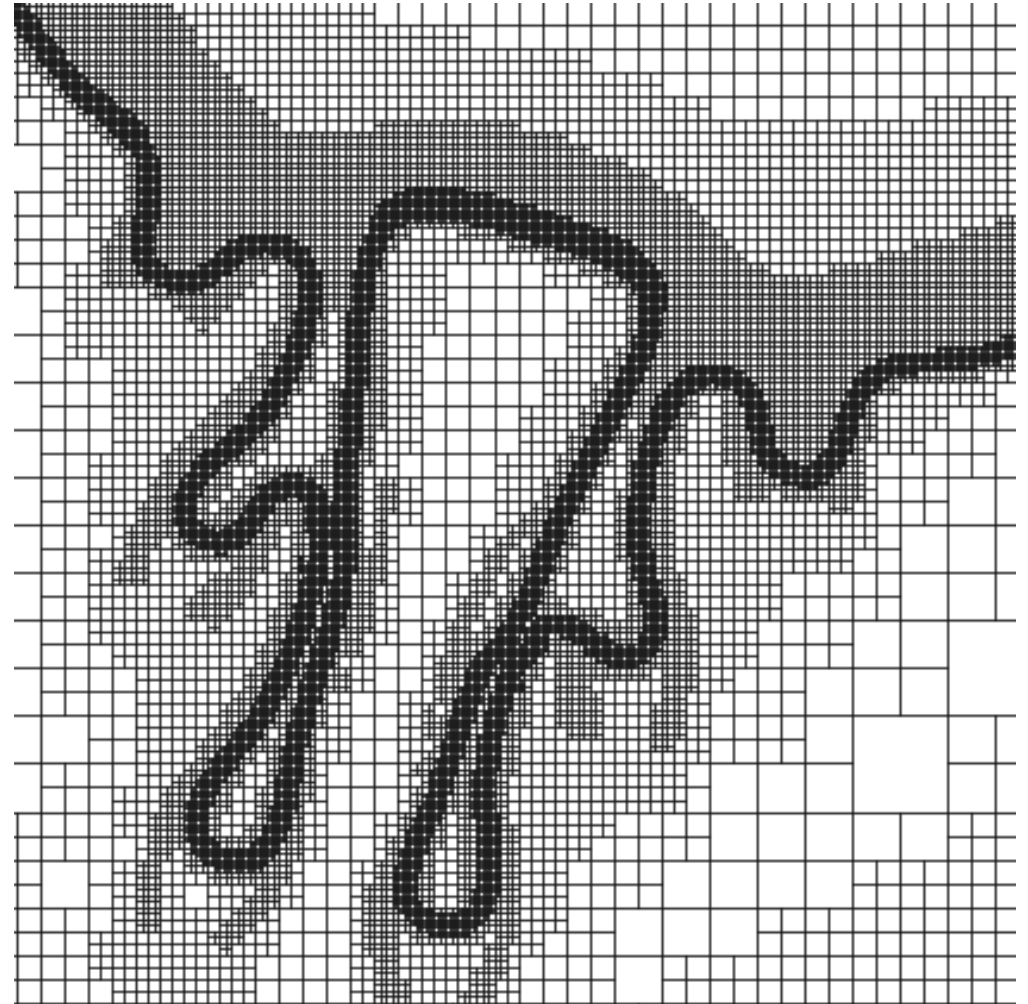
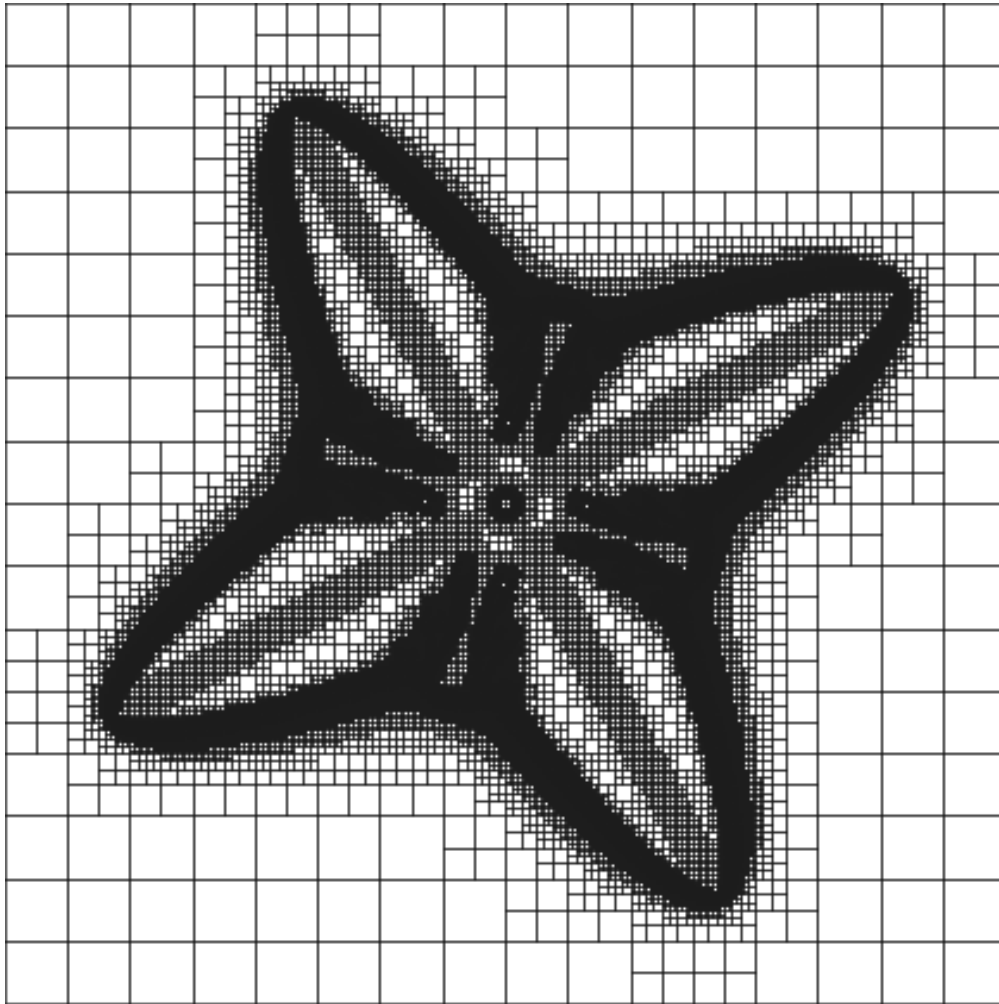


phase field



concentration field

FEM: Adaptive grid

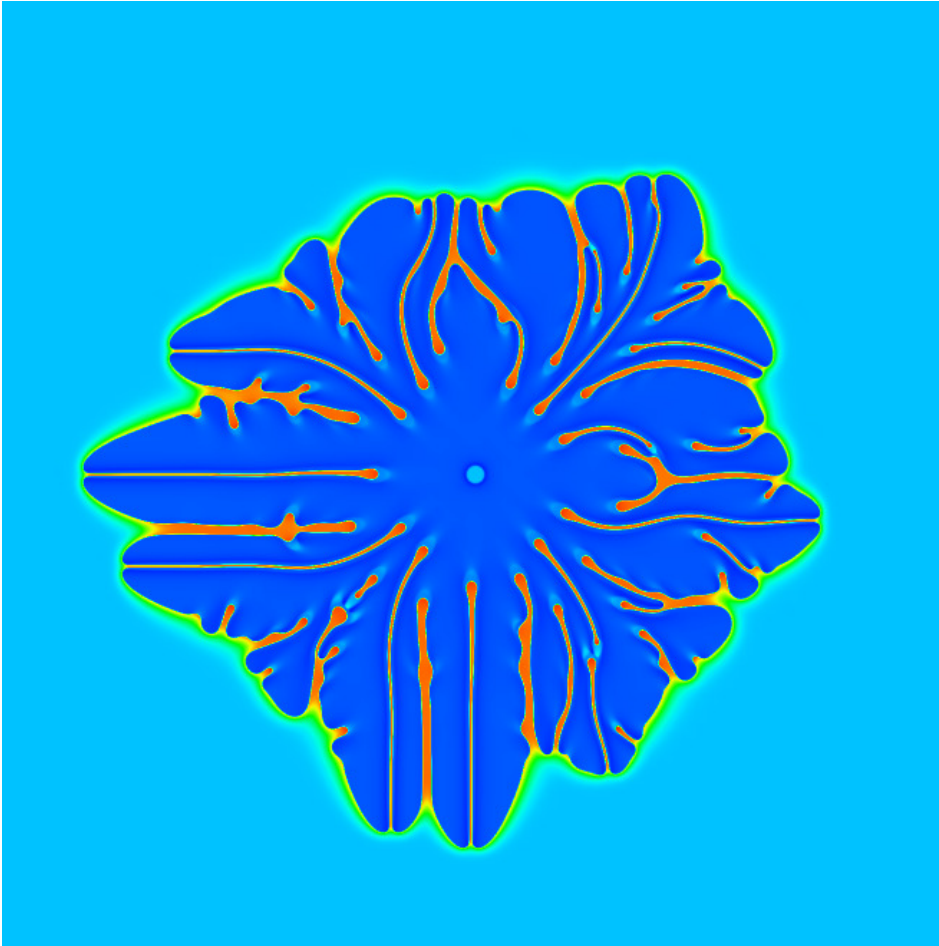


| ← L → |

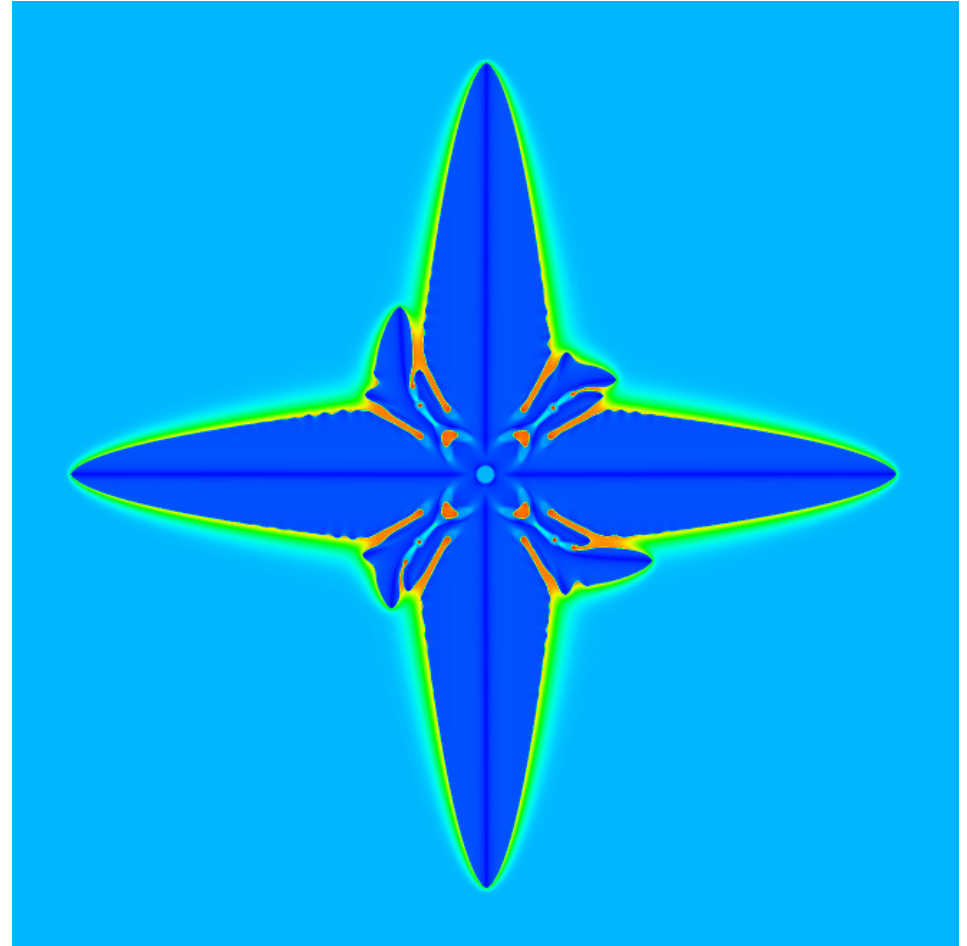
$$\frac{L}{\Delta x_{\min}} = 2048$$

Anisotropy of the interface

$$\text{gradient energy } a(\nabla\varphi) = \gamma(1 + \delta_\gamma \cos\beta)(\nabla\varphi)^2$$



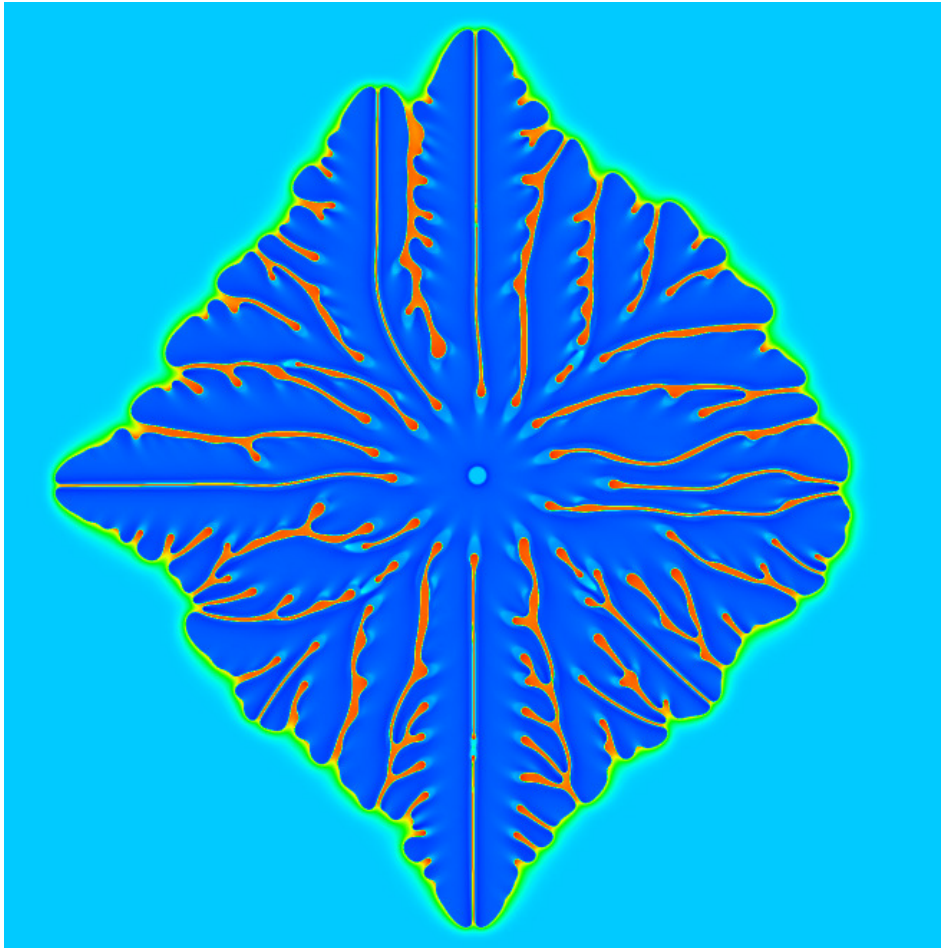
$$\delta_\gamma = 0$$



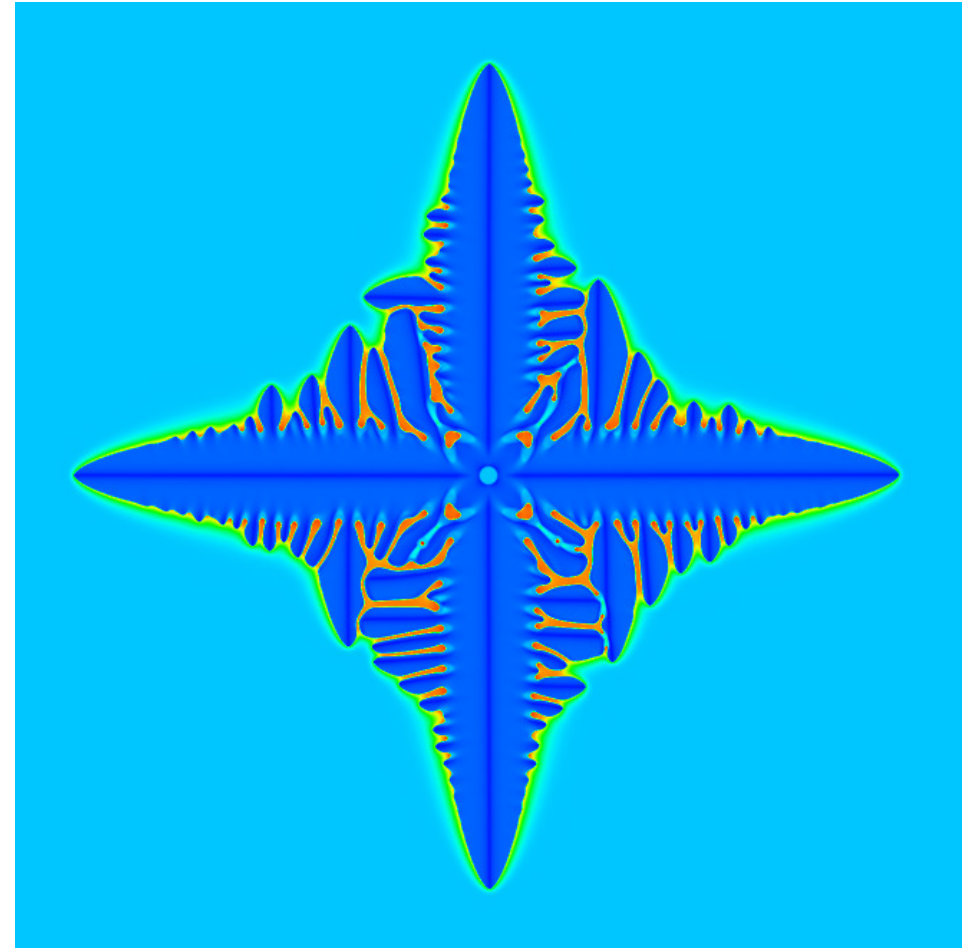
$$\delta_\gamma = 0.04$$

Noise

driving force $\rightarrow (1 + \alpha r) \times$ driving force, $-1 < r < +1$

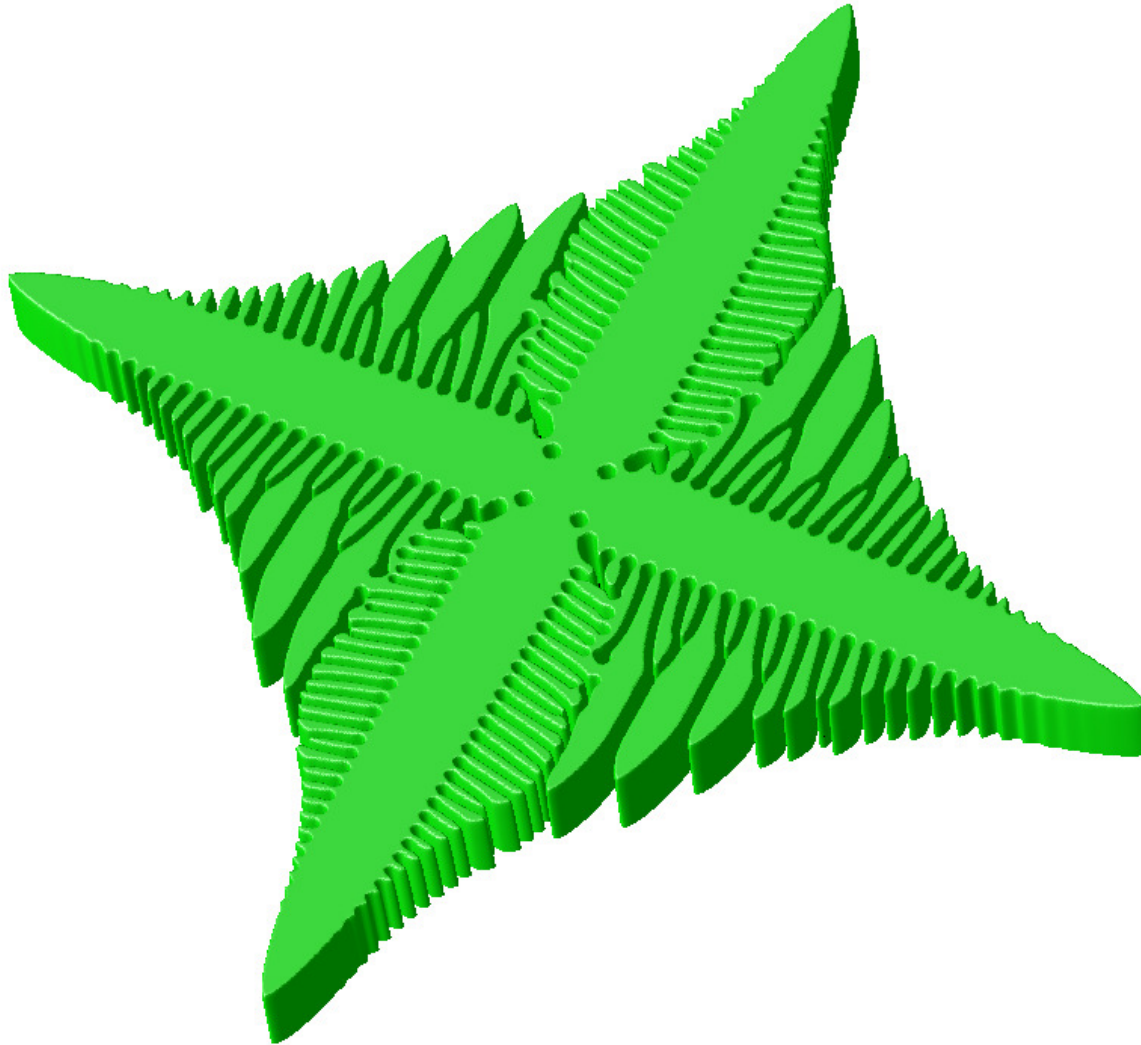


$$\delta_\gamma = 0, \alpha = 0.25$$



$$\delta_\gamma = 0.04, \alpha = 0.25$$

Further examples



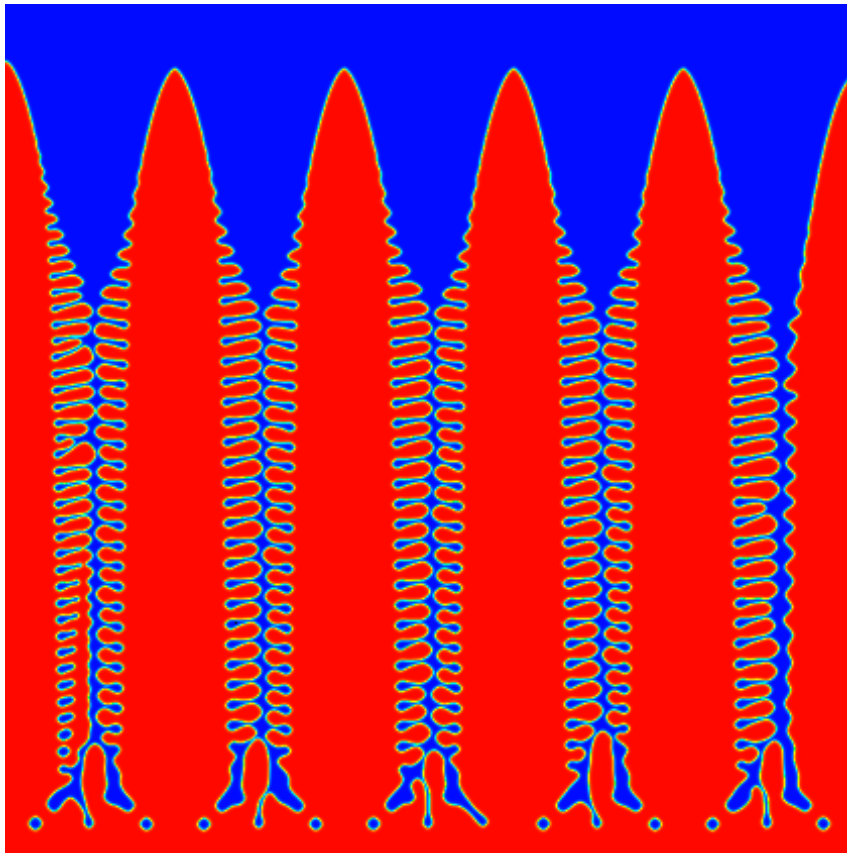
~80 h
(AMD Opteron)

10000 time steps

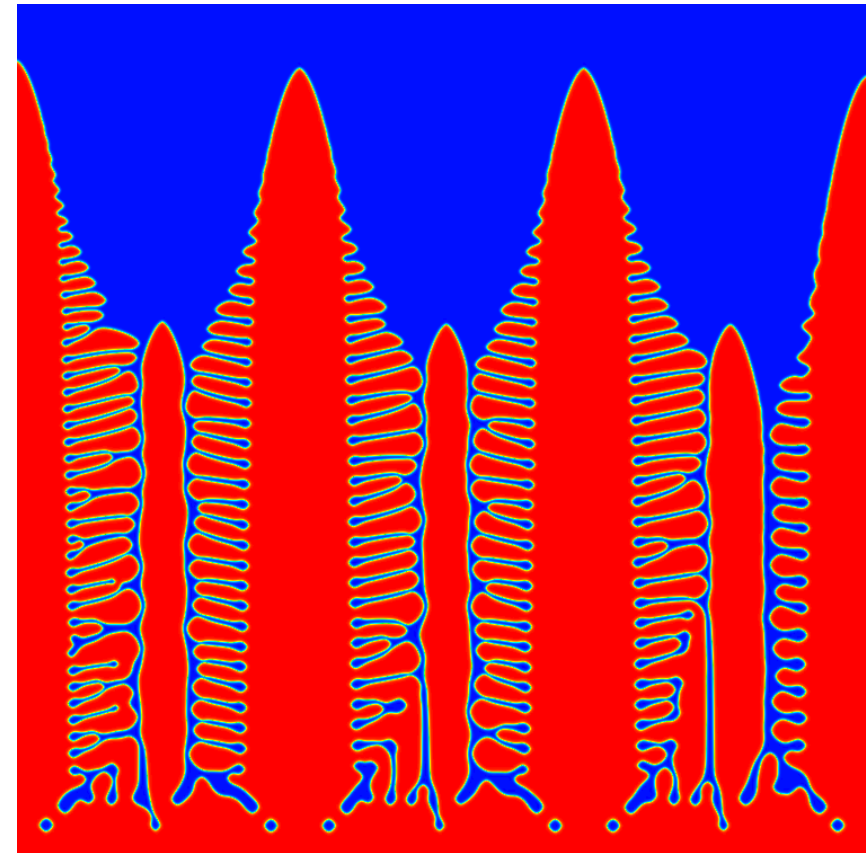
637 → 1140883
active cells

$$\frac{L}{\Delta x_{\min}} = 8192$$

Further examples



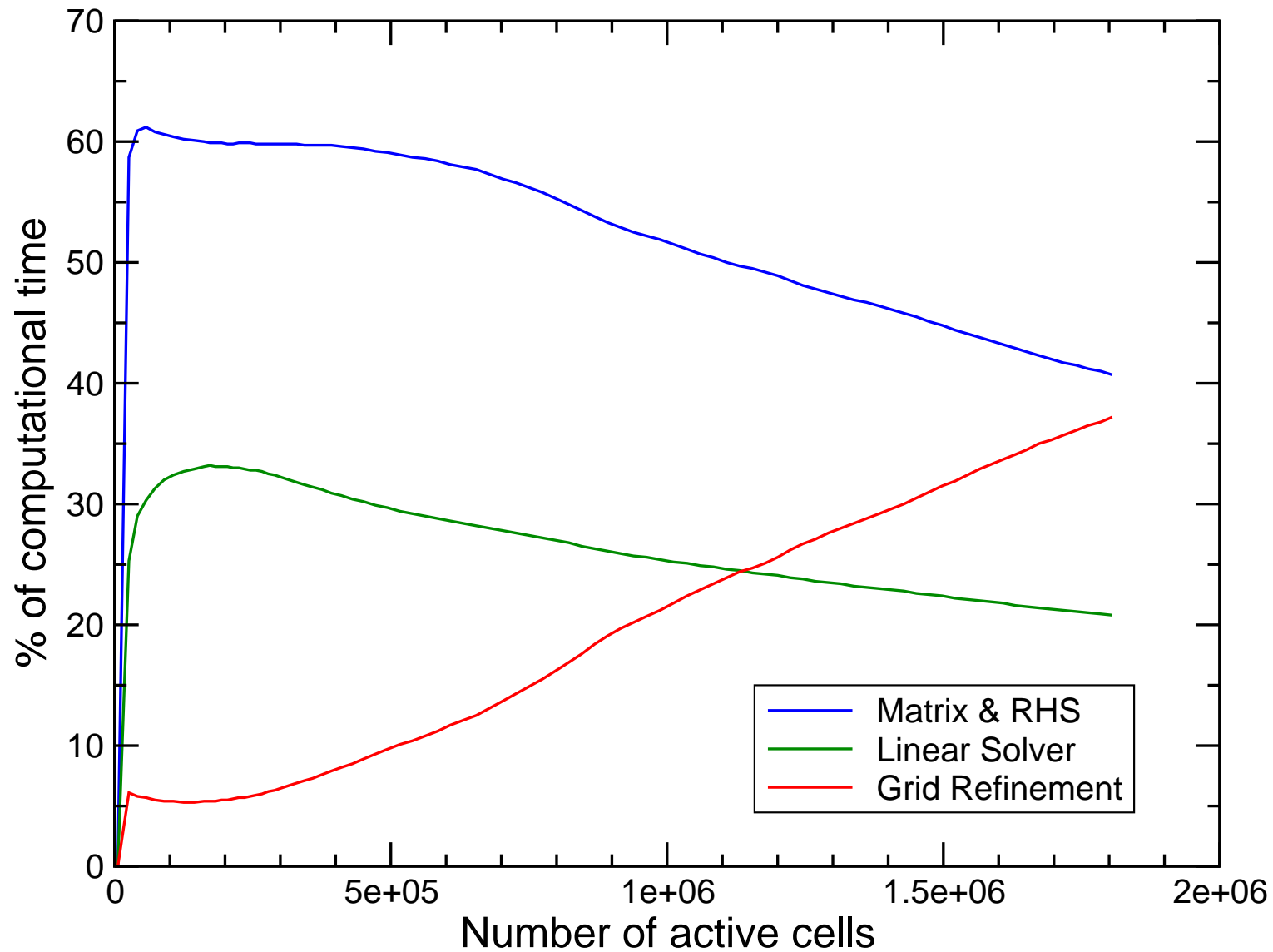
1 805 380 active cells



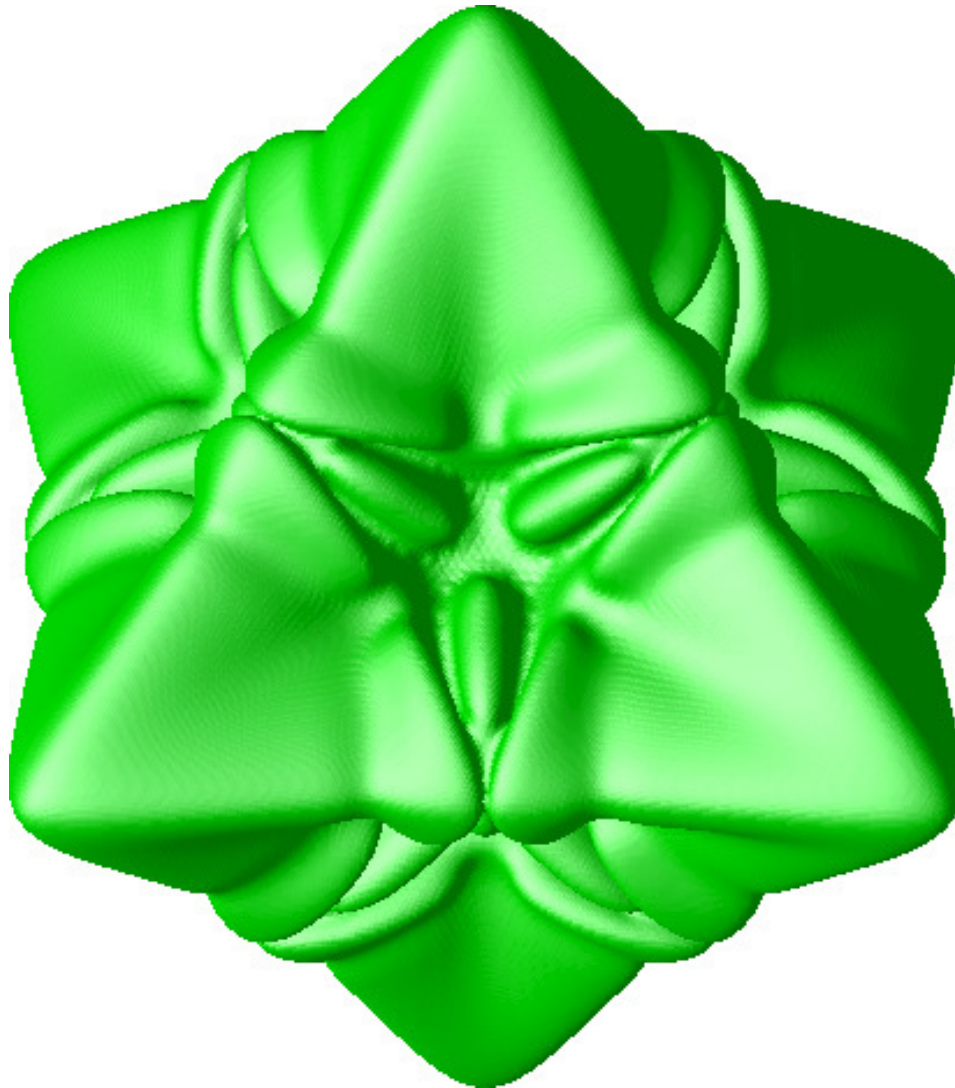
1 862 719 active cells

9000 time steps, $\frac{L}{\Delta x_{\min}} = 4096$

Further examples



Further examples



4600 time steps

1303 → 347992
active cells

$$\frac{L}{\Delta x_{\min}} = 256$$

Features request

- Periodic boundary conditions.
- Output to binary OpenDX-files.
- Platform-independent binary format in `Vector<Number>::block_write/block_read`.