Numerical Approximation of Facetted Pattern Formation in Snow Crystal Growth

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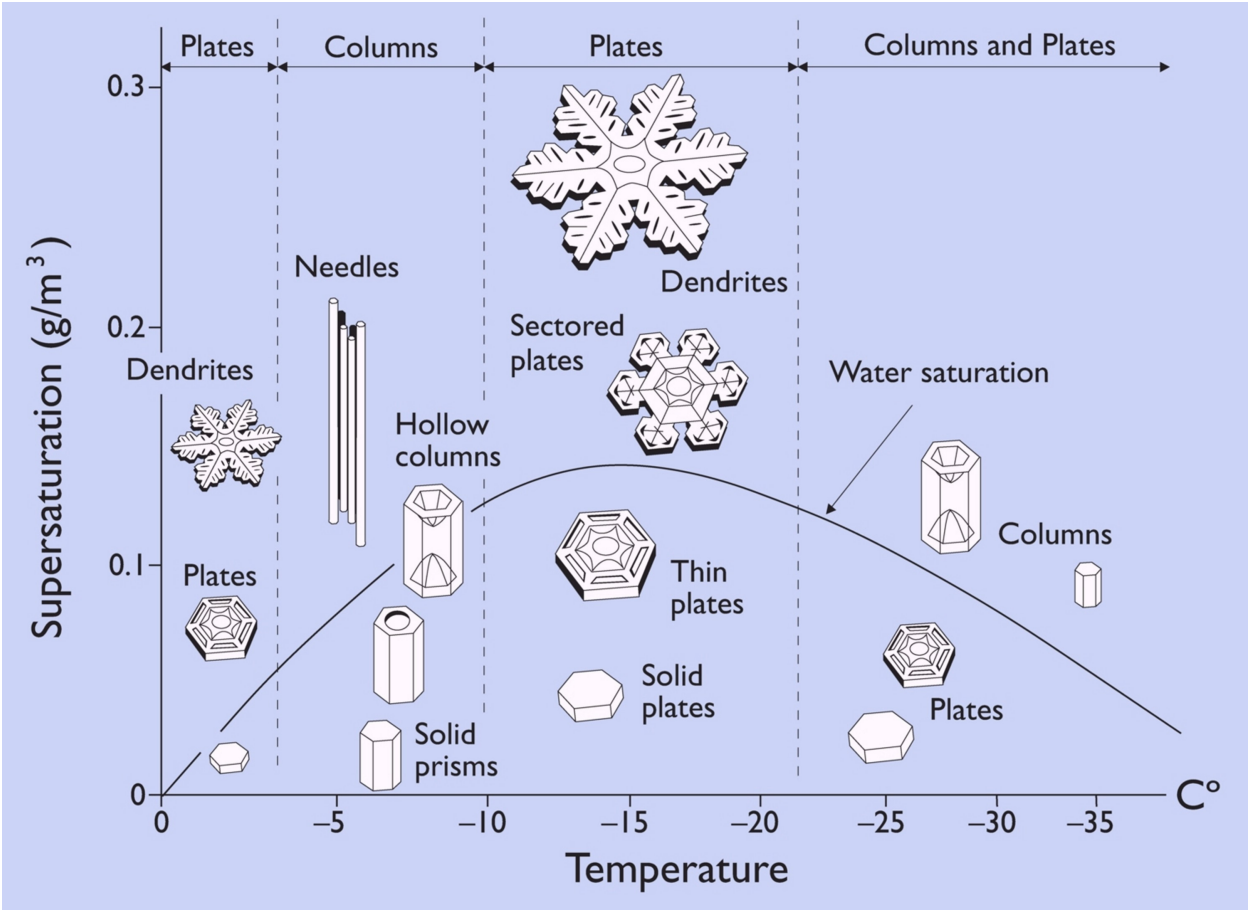
Snow crystals

Snowflake crystals come in many shapes and forms.

Their precise form depends in a very subtle way on the temperature and on the supersaturation (amount of excess water molecules).

U. Nakaya (1900-1962) analysed these dependencies and created his now famous Nakaya *snow crystal morphology diagram*.



Snow crystals

As a snow flake falls towards Earth, it experiences many different physical parameters.

All photos taken from www.SnowCrystals.com

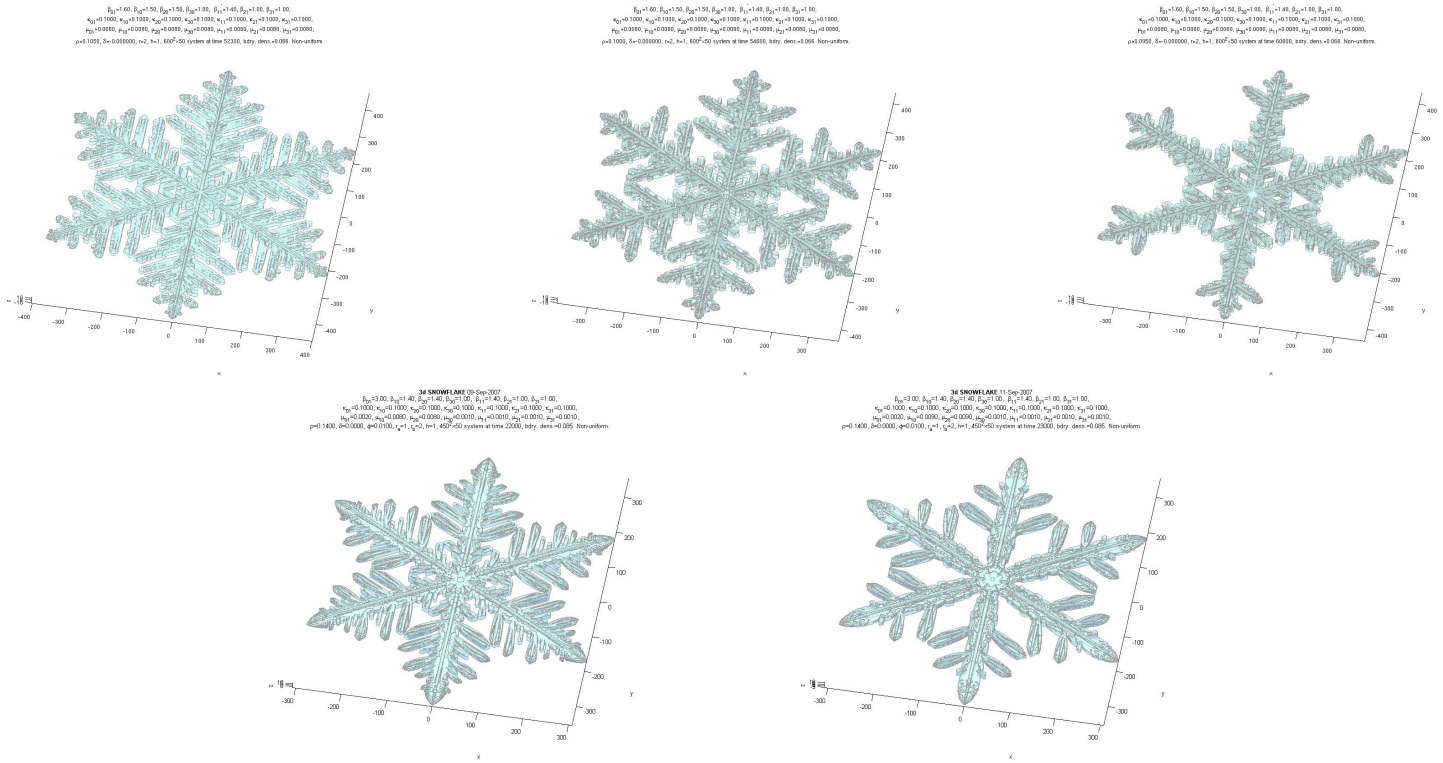
Nakaya called them "letters from the sky".

Introduction

The mathematical modelling and computational approximation of snow crystal growth is very challenging.

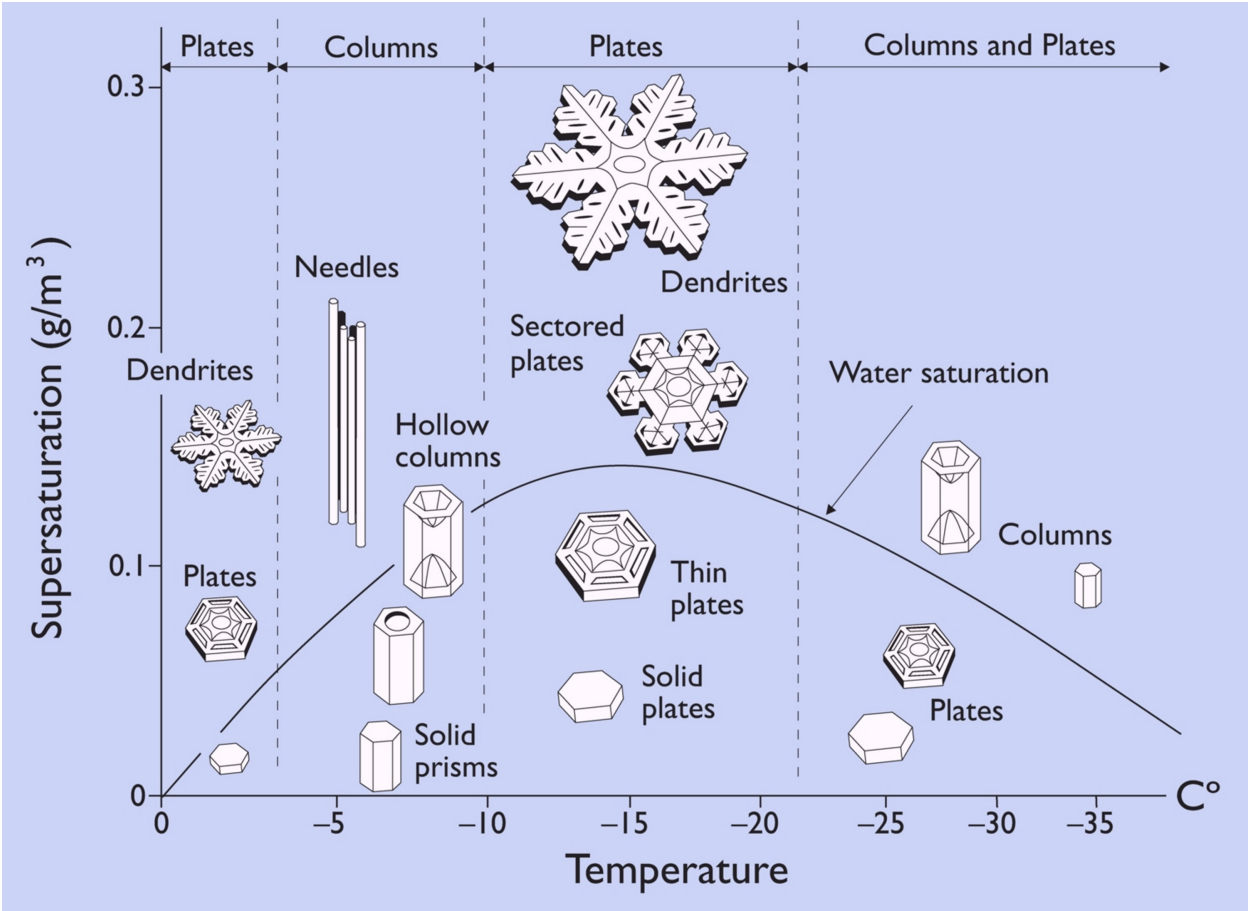
The most successful simulations of snow crystal growth so far are based on heuristic discrete models, so-called **cellular automata**.

See e.g. Gravner, Griffeath (09).



So far, there are no realistic numerical approximations for a **continuum model** of snow crystal growth.

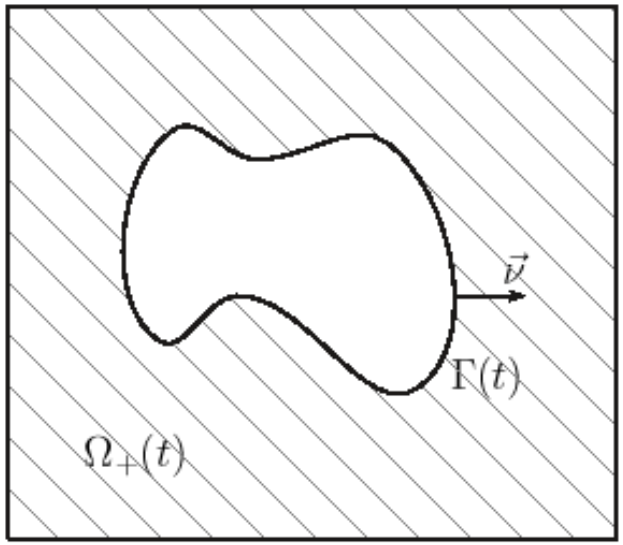
AIM: Develop a numerical approximation for such a continuum model that produces realistic snowflake morphologies.



A continuum model

A continuum model for an ice crystal growing from water vapour is given in Libbrecht (05).

Let Ω be a domain in $\mathbb{R}^d$, $d = 2$ or $d = 3$.



Let $\Omega_+(t) \subset \Omega$ denote the gas phase.

Let $\Gamma(t) := \partial\Omega_+(t) \setminus \partial\Omega$ denote the gas/solid interface.

Let $\vec{\nu}$ be the unit normal to $\Gamma(t)$ pointing into $\Omega_+(t)$.

Let c denote the water vapour number density in the gas phase $\Omega_+(t)$.

Diffusion equation in the gas phase:

$$c_t - \mathcal{D}\,\Delta\, c = 0 \quad \text{in} \quad \Omega_+(t)\,,$$

where $\mathcal{D} > 0$ is a diffusion constant.

A continuum model

Mass balance at gas/solid interface:

$$\mathcal{D}\,\frac{\partial c}{\partial \vec{\nu}} = (c_{\text{solid}} - c)\,\mathcal{V} \quad \text{on} \quad \Gamma(t)\,,$$

where $c_{\text{solid}} \approx 3 \times 10^{28}\,\text{m}^{-3}$ is the number density for ice, and $\mathcal{V}$ is the velocity of $\Gamma(t)$ in the direction $\vec{\nu}$. Note: $c \ll c_{\text{solid}}$.

Surface tension effects and attachment kinetics:

$$c = c_{\text{sat}}\,(1 - \delta\,\kappa_\gamma + \frac{\mathcal{V}}{\beta(\vec{\nu})\,v_{\text{kin}}}) \quad \text{on} \quad \Gamma(t)\,,$$

where $\delta = \widehat{\gamma}/(c_{\text{solid}}\,K\,T) \approx 1\,\text{nm}$ with

$\widehat{\gamma} \approx 0.1\,\text{Jm}^{-2}$	typical order of the surface tension of ice
$K \approx 1.4 \times 10^{-23}\,\text{JK}^{-1}$	the Boltzmann constant
T	temperature
v_{kin}	kinetic velocity
$c_{\text{sat}} = c_{\text{sat}}(T)$	equilibrium number density above a flat ice surface
κ_γ	anisotropic mean curvature
$\beta(\vec{\nu})$	condensation coefficient

Finally, we complement the system with the boundary conditions

$$c = c_{\text{sat}} + c_{\text{super}} \quad \text{on} \quad \partial\Omega\,.$$

A continuum model

$$
\begin{aligned}
c_t - \mathcal{D}\,\Delta\, c &= 0 && \text{in } \Omega_+(t)\,,\\
\mathcal{D}\,\frac{\partial c}{\partial \vec{\nu}} &= (c_{\text{solid}} - c)\,\mathcal{V} && \text{on } \Gamma(t)\,,\\
c &= c_{\text{sat}}\,(1 - \delta\,\kappa_\gamma + \frac{\mathcal{V}}{\beta(\vec{\nu})\,v_{\text{kin}}}) && \text{on } \Gamma(t)\,,\\
c &= c_{\text{sat}} + c_{\text{super}} && \text{on } \partial\Omega\,.
\end{aligned}
$$

In this simple model, energy balance and latent heat are neglected (as particle diffusion is much slower than heat diffusion). Moreover, the condensation coefficient β only depends on the local orientation of the growing crystal.

In reality, β is known to strongly depend on the temperature T, and possibly on c. However, the precise dependence is not known. But it is believed that certain physical phenomena can be encoded into the condensation coefficient: surface roughening, surface melting and kinetic roughening. See Libbrecht (05) for details.

Nevertheless, this simple model with reasonable choices for $\beta(\vec{\nu})$ allows the computation of a wide range of snowflake morphologies observed in reality.

Non-dimensionalization

As length scale we choose $R = 100\mu\text{m}$. As time scale we choose $\tilde{t} = \frac{R^2}{\mathcal{D}} \frac{c_{\text{solid}}}{c_{\text{sat}}}$.

Introducing the non-dimensionalized concentration

$$u = \frac{c - c_{\text{sat}}}{c_{\text{sat}}}$$

and rescaling $\vec{x} \to \vec{x}/R$, $t \to t/\tilde{t}$ we obtain, on recalling that $c, c_{\text{sat}} \ll c_{\text{solid}}$ the non-dimensionalized problem

$$\begin{aligned} -\Delta u &= 0 && \text{in } \Omega_+(t), \\ \frac{\partial u}{\partial \vec{\nu}} &= \mathcal{V} && \text{on } \Gamma(t), \\ \frac{\rho\,\mathcal{V}}{\beta(\vec{\nu})} &= \alpha\,\kappa_\gamma + u && \text{on } \Gamma(t), \end{aligned}$$

where $\rho := (\mathcal{D}\, c_{\text{sat}})/(R\, c_{\text{solid}}\, v_{\text{kin}}) \approx 1.42 \times 10^{-3}$ for values of T between $-1°\text{C}$ and $-30°\text{C}$, and $\alpha := \delta/R \approx 10^{-5}$. See Libbrecht (05).

Varying $\beta = \beta(\cdot, T)$ and the boundary conditions

$$u = u_{\partial\Omega} := \frac{c_{\text{super}}}{c_{\text{sat}}} \quad \text{on } \partial\Omega$$

models different choices for temperature and supersaturation.

Anisotropy

The anisotropic mean curvature κ_γ can be introduced as follows.

The total surface energy of an interface Γ is given by the surface integral

$$\int_\Gamma \gamma(\vec{\nu})\, \mathrm{d}s\,.$$

Here $\gamma(\vec{\nu})$ encodes the effect of the underlying crystal structure.

The first variation of the above energy can now be computed as

$$\kappa_\gamma := -\nabla_s \cdot \gamma'(\vec{\nu})\,,$$

see e.g. Cahn, Hoffmann (74).

Here, for mathematical convenience, we have defined

$$\gamma(\vec{p}) := |\vec{p}|\, \gamma(\frac{\vec{p}}{|\vec{p}|}) \qquad \forall\ 0 < |\vec{p}| \neq 1\,.$$

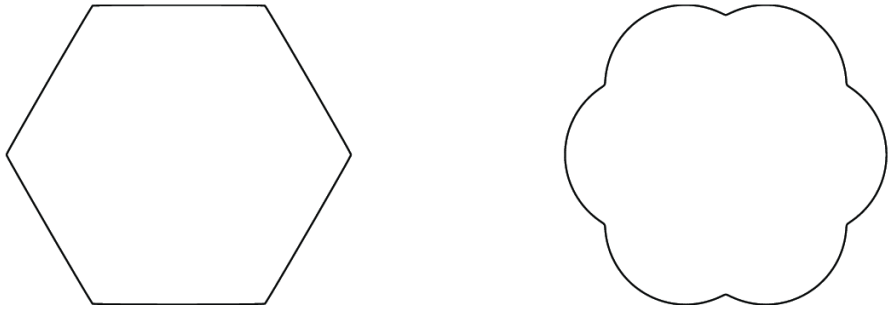
I.e. κ_γ measures how much $\int_\Gamma \gamma(\vec{\nu})\, \mathrm{d}s$ changes if Γ is changed locally in the direction of $\vec{\nu}$.

Anisotropy

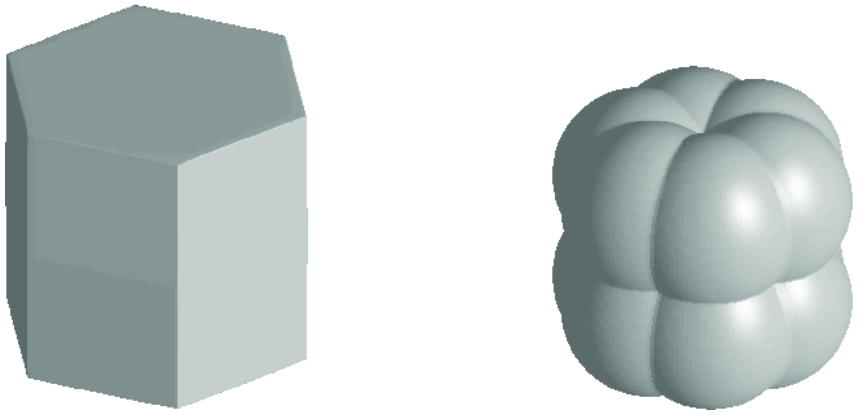
Relevant for the modelling of snow crystal growth are hexagonal surface energy anisotropies.

Example Wulff shapes $\mathcal{W}$ (scaled surface area minimiziers) and polar plots $\mathcal{P} := \{\gamma(\vec{p})\,\vec{p} : |\vec{p}| = 1\}$ are given below.

2d:



3d:



Mathematical problem

We want to numerically approximate: For all $t \geq 0$ find $\Gamma(t) = \partial\Omega_+(t) \setminus \partial\Omega \subset \Omega$ and $u(\cdot, t) : \Omega_+(t) \to \mathbb{R}$ such that

$$
\begin{aligned}
-\Delta u &= 0 && \text{in } \Omega_+(t), \\
\frac{\partial u}{\partial \vec{\nu}} &= \mathcal{V} && \text{on } \Gamma(t), \\
\frac{\rho\,\mathcal{V}}{\beta(\vec{\nu})} &= \alpha\,\kappa_\gamma + u && \text{on } \Gamma(t), \\
u &= u_{\partial\Omega} && \text{on } \partial\Omega\,.
\end{aligned}
$$

This is a **one-sided** Stefan/Mullins–Sekerka problem with anisotropic Gibbs–Thomson law and kinetic undercooling.

Challenges:

(1) Given $\Omega_+(t)$ and $\mathcal{V}$, solve an elliptic problem with Neumann data on a curved boundary for u.

(2) Given u, solve a forced geometric evolution equation for $\Gamma(t)$.

(3) Incorporate the nearly crystalline, hexagonal anisotropy.

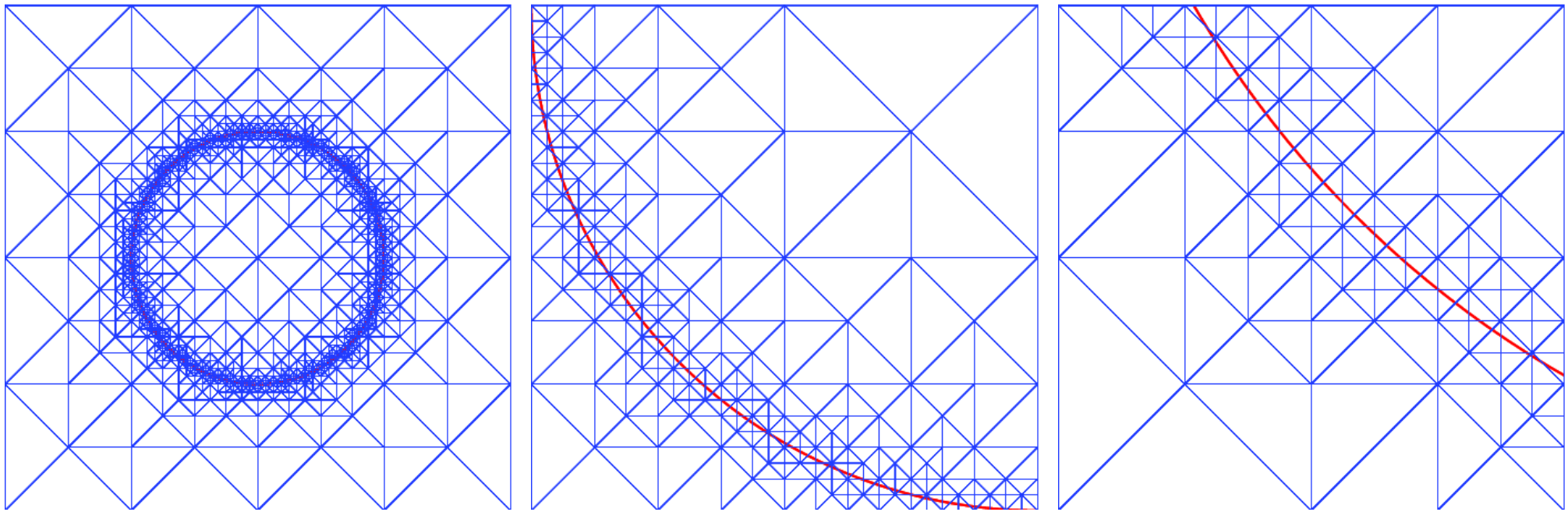
(4) Coupling of the problems for u and $\Gamma(t)$.

Challenge (1)

$$
\begin{aligned}
-\Delta u &= 0 \qquad && \text{in } \Omega_+(t), \\
\frac{\partial u}{\partial \vec{\nu}} &= \mathcal{V} \qquad && \text{on } \Gamma(t).
\end{aligned}
$$

(1) Given $\Omega_+(t)$ and $\mathcal{V}$, solve an elliptic problem with Neumann data on a curved boundary for u.

Here we employ an **unfitted** finite element method, as in Barrett, Elliott (84); together with local mesh refinement.



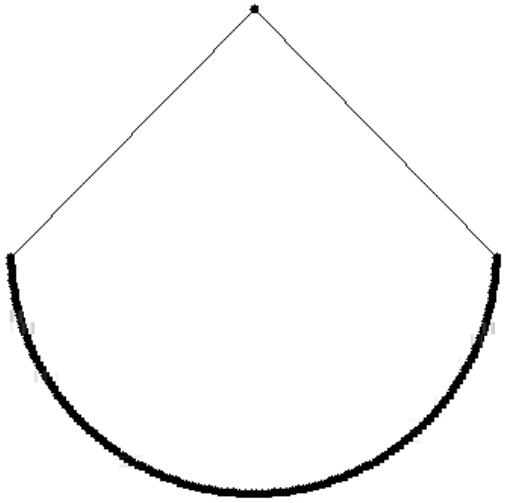
Challenge (2)

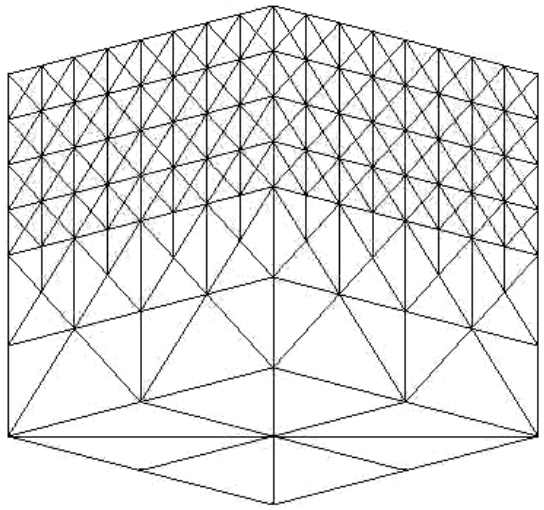
$$\mathcal{V} = \mathcal{F}(\kappa_\gamma, u) \qquad \text{on} \quad \Gamma(t).$$

(2) Given u, solve a forced geometric evolution equation for $\Gamma(t)$.

For simplicity, replace κ_γ with the (isotropic) mean curvature κ. Then we can use the parametric finite element approximations from Barrett, Garcke, Nürnberg (08a) $\Rightarrow$ **no remeshing needed**.

Example: $\mathcal{F}(\kappa, u) = -\Delta_s \kappa$ (surface diffusion)

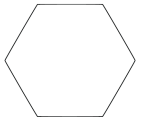


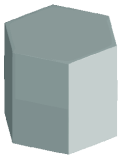


Challenge (3)

$$\frac{\rho\,\mathcal{V}}{\beta(\vec{\nu})} = \alpha\,\kappa_\gamma + u \qquad \text{on} \quad \Gamma(t)$$

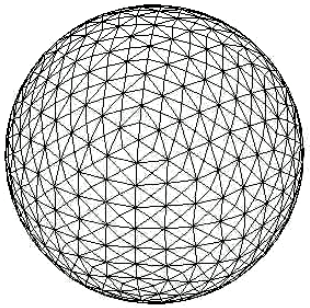
(3) Incorporate the nearly crystalline, hexagonal anisotropy:

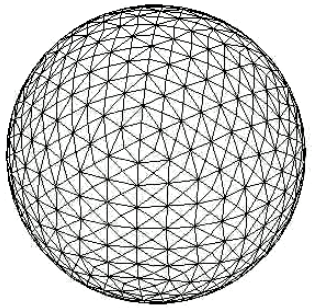




Using ideas from differential geometry, Barrett, Garcke, Nürnberg (08b) reformulated the anisotropic mean curvature κ_γ in a way that lends itself to a **stable variational approximation**.

Example: $\mathcal{F}(\kappa_\gamma, u) = -\Delta_s\,\kappa_\gamma$ (anisotropic surface diffusion)





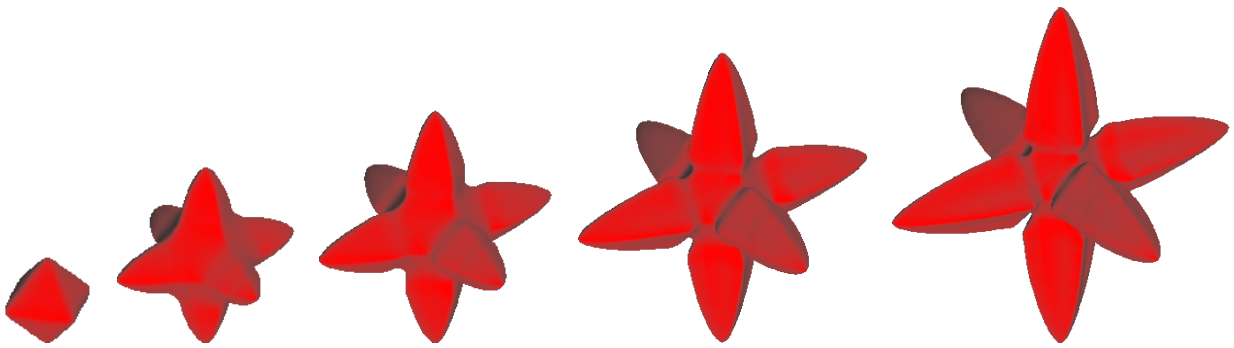
Challenge (4)

$$
\begin{aligned}
-\Delta u &= 0 && \text{in } \Omega_+(t),\\
\frac{\partial u}{\partial \vec{\nu}} &= \mathcal{V} && \text{on } \Gamma(t),\\
\frac{\rho\,\mathcal{V}}{\beta(\vec{\nu})} &= \alpha\,\kappa_\gamma + u && \text{on } \Gamma(t).
\end{aligned}
$$

(4) Coupling of the problems for u and $\Gamma(t)$.

Here we employ a variational formulation that respects the underlying energy structure of the continuous problem.

One-sided analogoue of the finite element method for the two-sided Stefan/ Mullins–Sekerka problems introduced in Barrett, Garcke, Nürnberg (10).



Let

$$S_{0,+}(t) := \{\phi \in H^1(\Omega_+(t)) : \phi = 0 \quad \text{on } \partial\Omega\}$$
$$\text{and} \quad S_{D,+}(t) := \{\phi \in H^1(\Omega_+(t)) : \phi = u_{\partial\Omega} \quad \text{on } \partial\Omega\}\,.$$

In addition, let

$$\underline{V} := H^1(\Upsilon, \mathbb{R}^d) \quad \text{and} \quad W := H^1(\Upsilon, \mathbb{R})\,,$$

where Υ is a reference manifold for $\Gamma(t)$.

Find $u(\cdot,t) \in S_{D,+}(t)$, $\Gamma(t) = \vec{x}(\Upsilon,t)$ with $\vec{x}(\cdot,t) \in \underline{V}$, and $\kappa_\gamma(\cdot,t) \in W$ such that

$$\int_{\Omega_+(t)} \nabla u \,.\, \nabla \phi \,\mathrm{d}x = -\int_{\Gamma(t)} \vec{x}_t \,.\, \vec{\nu}\, \phi \,\mathrm{d}s \qquad \forall\ \phi \in S_{0,+}(t)\,,$$
$$\rho \int_{\Gamma(t)} \frac{\vec{x}_t \,.\, \vec{\nu}\, \chi}{\beta(\vec{\nu})} \,\mathrm{d}s = \int_{\Gamma(t)} [\alpha\, \kappa_\gamma + u]\, \chi \,\mathrm{d}s \qquad \forall\ \chi \in W\,,$$
$$\int_{\Gamma(t)} \kappa_\gamma\, \vec{\nu} \,.\, \vec{\eta} \,\mathrm{d}s + \langle \nabla_s^{\widetilde{G}}\, \vec{x}, \nabla_s^{\widetilde{G}}\, \vec{\eta} \rangle_\gamma = 0 \qquad \forall\ \vec{\eta} \in \underline{V}\,.$$

The inner product $\langle \nabla_s^{\widetilde{G}}\, \cdot, \nabla_s^{\widetilde{G}}\, \cdot \rangle_\gamma$ was introduced in BGN (08b).

Energy structure

The Lyapunov structure

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\alpha\int_{\Gamma(t)}\gamma(\vec{\nu})\,\mathrm{d}s+u_{\partial\Omega}\,\mathrm{vol}(\Omega_+(t))\right)+(\nabla u,\nabla u)_+ +\rho\int_{\Gamma(t)}\frac{\mathcal{V}^2}{\beta(\vec{\nu})}\,\mathrm{d}s=0\,,$$

is mimicked on the discrete level by our finite element approximation.

Let Γ^0, an approximation to $\Gamma(0)$. For $m\geq 0$, find $U^{m+1}\in S^m_{D,+}$, $\vec{X}^{m+1}\in \underline{V}(\Gamma^m)$ and $\kappa_\gamma^{m+1}\in W(\Gamma^m)$ such that for all $\varphi\in S^m_{0,+}$, $\chi\in W(\Gamma^m)$, $\vec{\eta}\in\underline{V}(\Gamma^m)$

$$(\nabla U^{m+1},\nabla\varphi)_{m,+}-\left\langle\pi^m\left[\frac{\vec{X}^{m+1}-\vec{X}^m}{\tau_m}\,.\,\vec{\omega}^m\right],\varphi\right\rangle_m=0\,,$$

$$\rho\left\langle[\beta(\vec{\nu}^m)]^{-1}\,\frac{\vec{X}^{m+1}-\vec{X}^m}{\tau_m},\chi\,\vec{\omega}^m\right\rangle_m^h-\alpha\,\langle\kappa_\gamma^{m+1},\chi\rangle_m^h-\langle U^{m+1},\chi\rangle_m=0\,,$$

$$\langle\kappa_\gamma^{m+1}\,\vec{\omega}^m,\vec{\eta}\rangle_m^h+\langle\nabla_s^{\widetilde{G}}\,\vec{X}^{m+1},\nabla_s^{\widetilde{G}}\,\vec{\eta}\rangle_{\gamma,m}=0\,;$$

and set $\Gamma^{m+1}=\vec{X}^{m+1}(\Gamma^m)$. Here we define

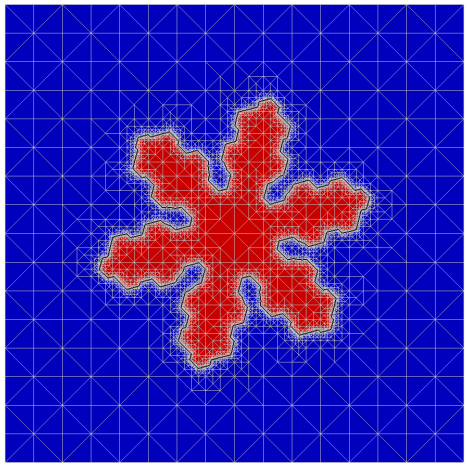
$$(\nabla\chi,\nabla\varphi)_{m,+}:=\int_{\Omega_+^{m,h}}\nabla\chi\,.\,\nabla\varphi\,\mathrm{d}x=\sum_{j=1}^{J_\Omega^m}\frac{|o_j^m\cap\Omega_+^{m,h}|}{|o_j^m|}\int_{o_j^m}\nabla\chi\,.\,\nabla\varphi\,\mathrm{d}x\,.$$

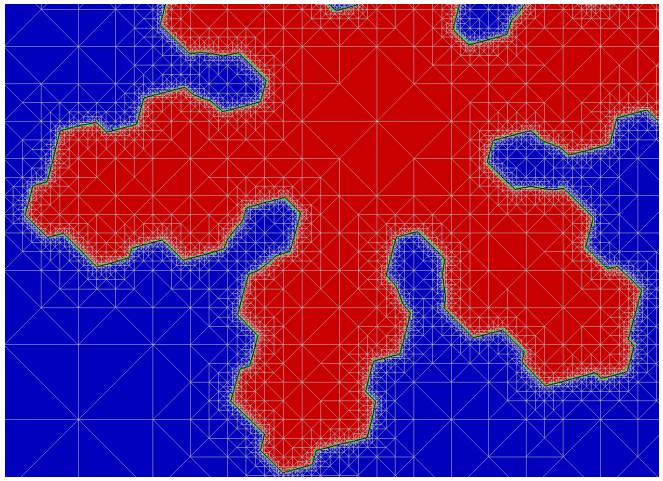
Linear system. Existence, uniqueness and stability.

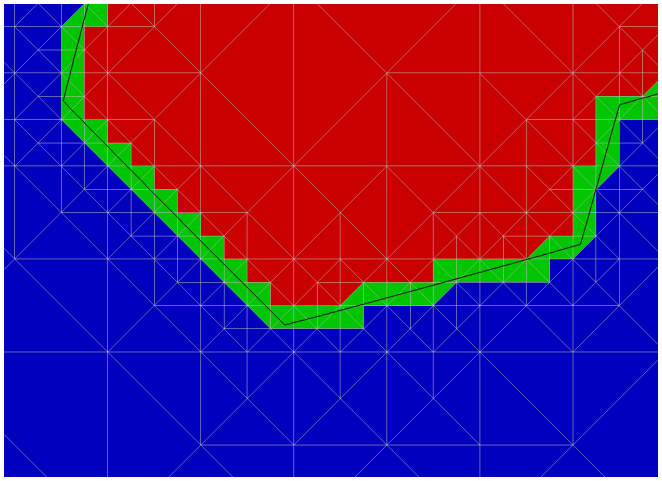
Evaluation of cross terms such as $\langle U^{m+1}, \chi \rangle_m$ requires computation of intersections between bulk mesh and interface mesh.

In addition, for the definition of $S^m_{D,+}$ and for the evaluation of the inner product $(\nabla U^{m+1}, \nabla \varphi)_{m,+}$ we have to define a discrete approximation $\Omega^{m,h}_+$ to the exact exterior Ω^m_+ of Γ^m in Ω.

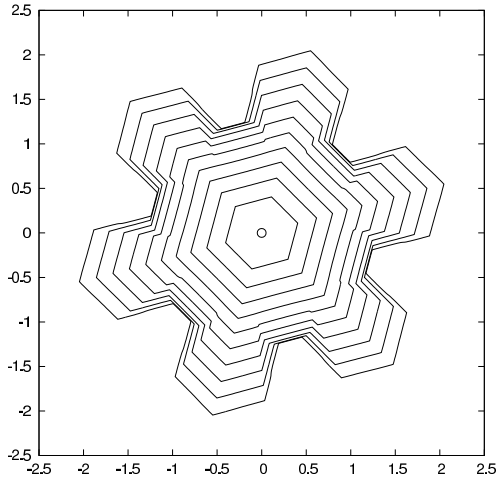
To this end, each element has to be marked as either belonging to Ω^m_+, or belonging to $\Omega \setminus \Omega^m_+$, or as being cut by Γ^m.



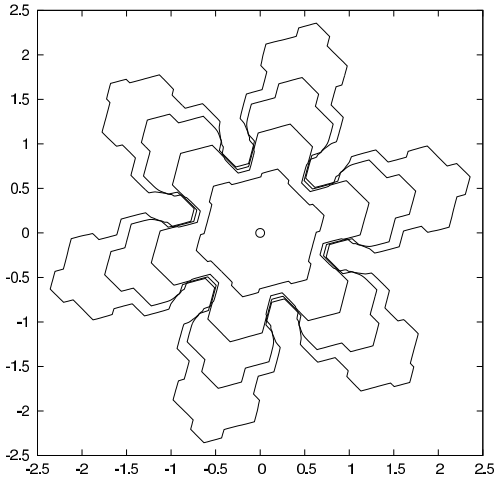




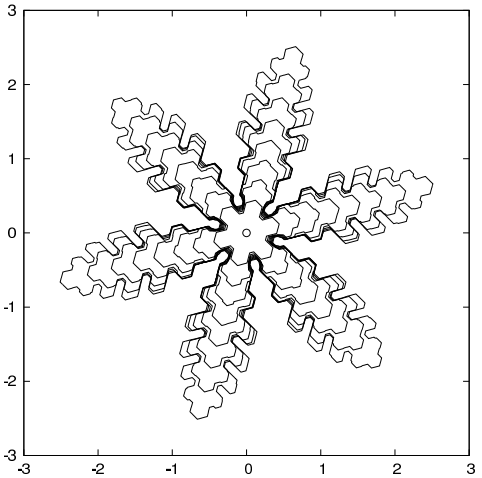
Numerical Results – 2d



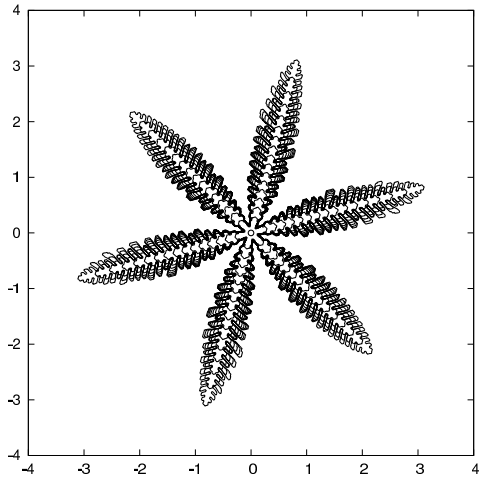
$u_{\partial\Omega} = 0.004$



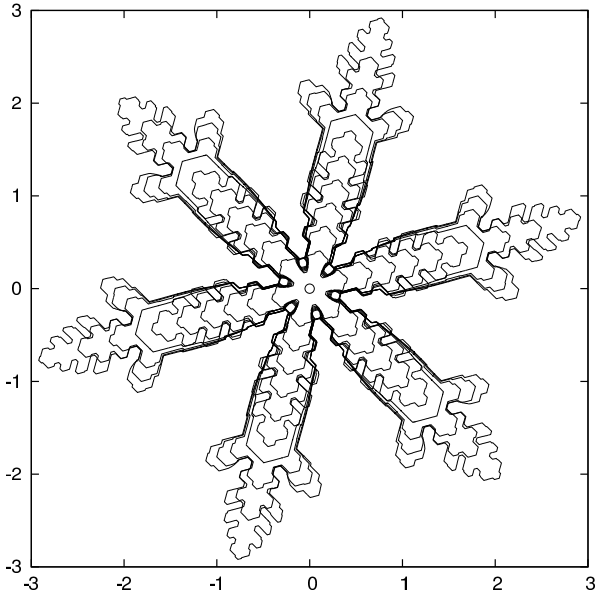
$u_{\partial\Omega} = 0.01$



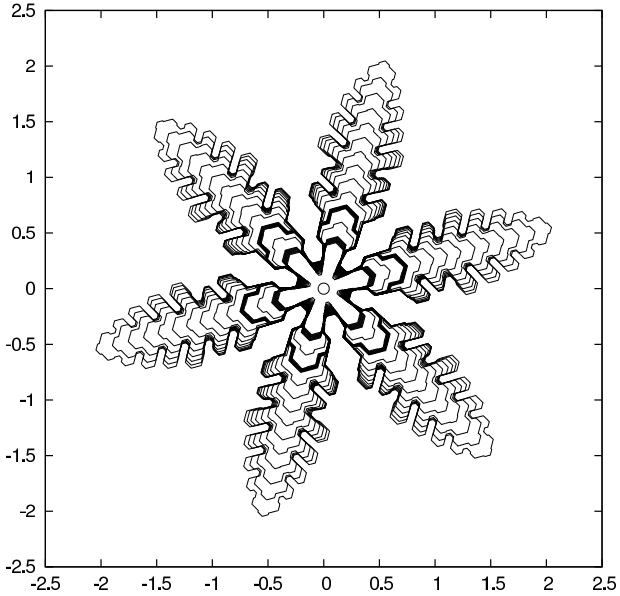
$u_{\partial\Omega} = 0.04$



$u_{\partial\Omega} = 0.2$



$u_{\partial\Omega} = [0.08\,|\,0.004\,|\,0.08]$



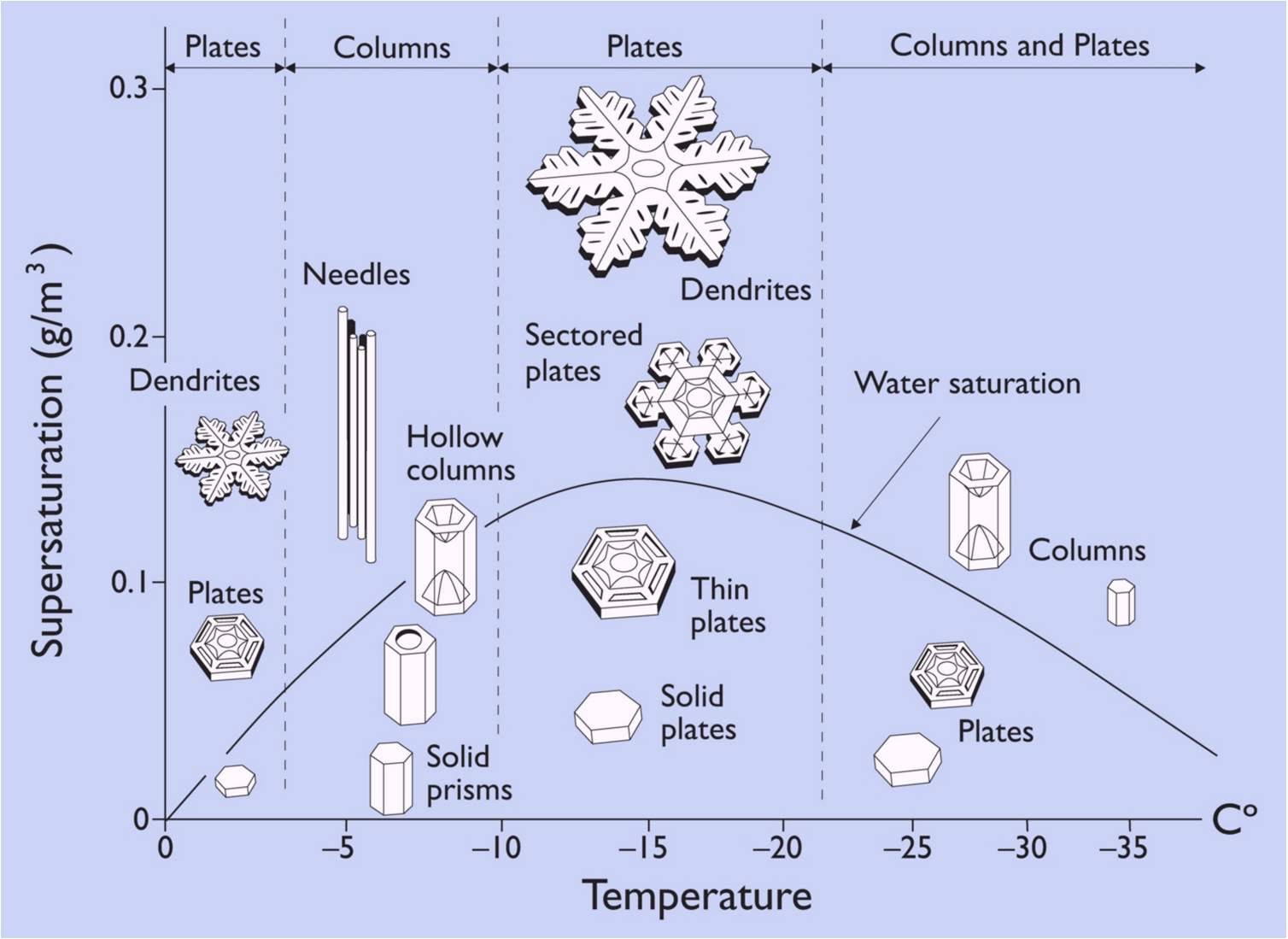
$u_{\partial\Omega} = [0.2\,|\,0.4\,|\,0.08\,|\,0.004\,|\,0.08\,|\,0.004\,|\,0.08]$

Numerical Results – 3d

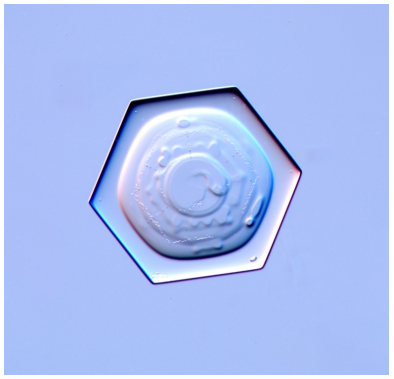
$$\rho\,\mathcal{V} = \beta(\vec{\nu})\,[\alpha\,\kappa_\gamma + u] \qquad \text{on} \quad \Gamma(t)$$

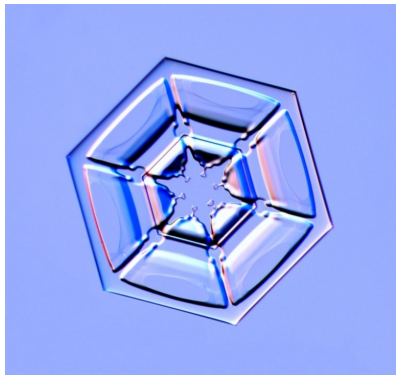
Define $\beta_{\text{flat},\ell}(\vec{p}) := [p_1^2 + p_2^2 + 10^{-2\ell}\,p_3^2]^{\frac{1}{2}}$ (to encourage *flat* growth),

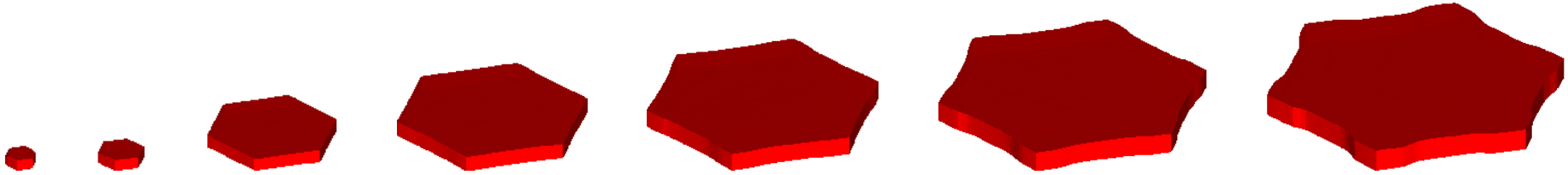
and $\beta_{\text{tall},\ell}(\vec{p}) := [10^{-2\ell}\,(p_1^2 + p_2^2) + p_3^2]^{\frac{1}{2}}$ (to encourage *tall* growth).



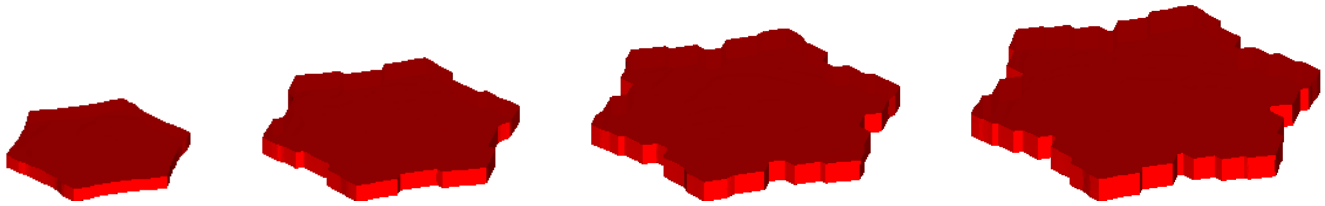
Numerical Results – 3d





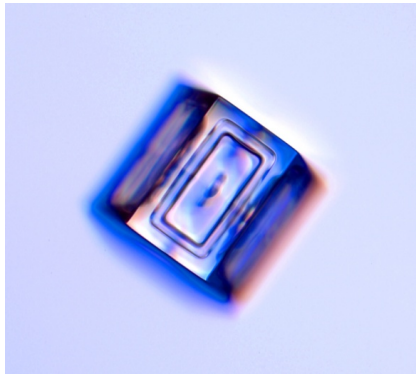


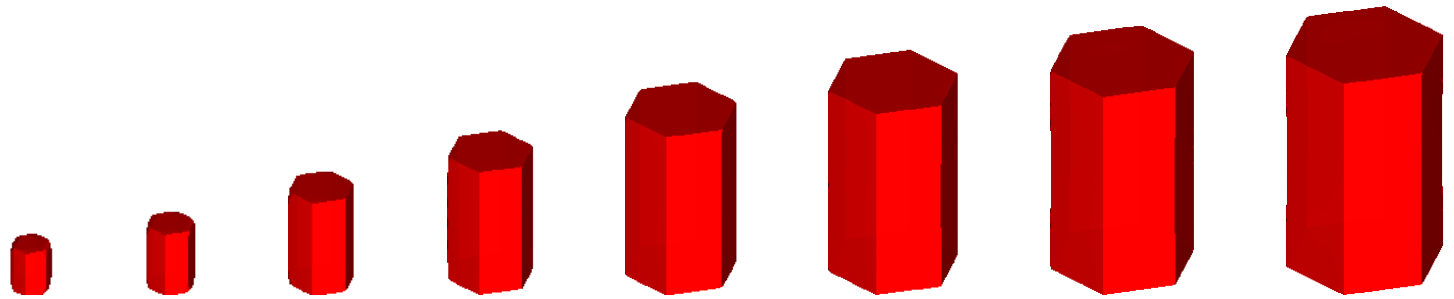
Solid plates. ($u_{\partial\Omega} = 0.004$, $\beta = \beta_{\text{flat},3}$)



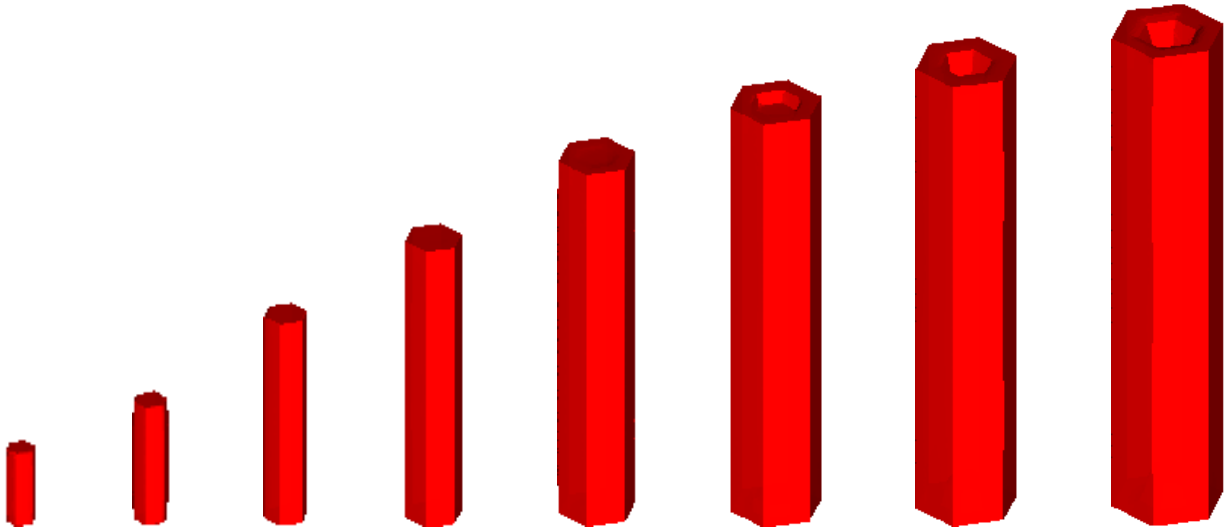
Dendrites. ($u_{\partial\Omega} = 0.004$, $\beta = \beta_{\text{flat},3}$)

Numerical Results – 3d



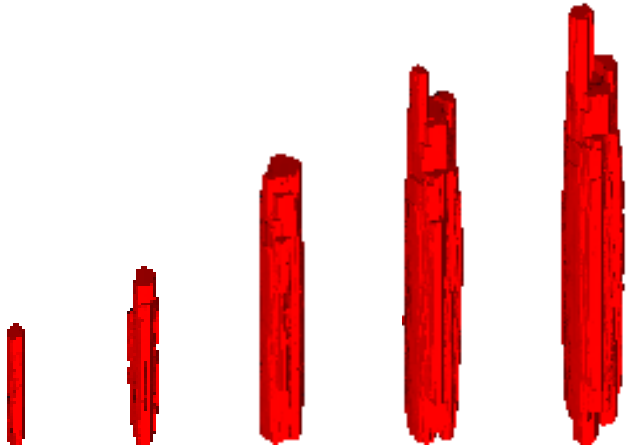


Solid prisms. ($u_{\partial\Omega} = 0.002$, $\beta = \beta_{\text{tall},1}$)

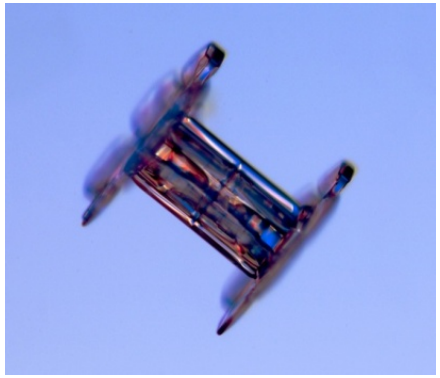


Hollow columns. ($u_{\partial\Omega} = 0.008$, $\beta = \beta_{\text{tall},2}$)

Numerical Results – 3d



Needles. ($u_{\partial\Omega} = 0.004$, $\beta = \beta_{\text{tall},3}$)



Capped columns. ($u_{\partial\Omega} = 0.02$, $\beta = \beta_{\text{flat},3}$)

Numerical Results – 3d

Sectored plates. ($u_{\partial\Omega} = [\,0.004\,|\,0.024\,|\,0.004\,]$, $\beta = \beta_{\text{flat},3}$)

Scrolls on plates. ($u_{\partial\Omega} = 0.004$, $\beta = [\,\beta_{\text{flat},3}\,|\,\beta_{\text{tall},3}\,]$)

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2. ——, *A variational formulation of anisotropic geometric evolution equations in higher dimensions*, Numer. Math., **109** (2008b), pp. 1–44.

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6. K. G. Libbrecht, *The physics of snow crystals*, Rep. Progr. Phys., **68** (2005), pp. 855–895.