The Stefan problem with anisotropic Gibbs–Thomson law

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Outline

1. Introduction
2. Anisotropic energies and weak formulation
3. Main existence result
4. Computational results

Stefan problem models

melting and solidification

Gibbs Thomson law

accounts for surface energy

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melting and solidification

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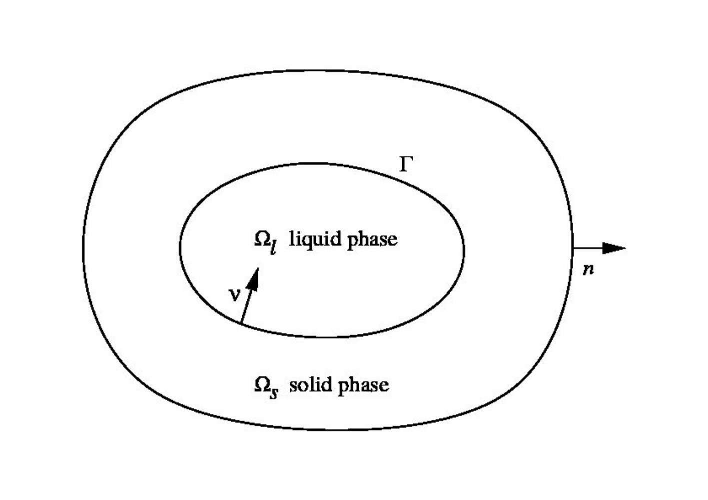
Geometry:



Mathematical description

Energy balance

$$\partial_t(u+\chi) - \Delta u = f \qquad \text{weakly !}$$

u : temperature
χ : characteristic function of liquid
f : heat sources

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Strong formulation:

in bulk	$\partial_t u - \Delta u = f$	heat equation
on interface Γ	$\mathcal{V} = -[\frac{\partial u}{\partial \nu}]$	Stefan condition

$\mathcal{V}$: normal velocity
$[.]$: jump across interface

Further condition on interface

Classical condition

$$u = 0 \quad (= \text{melting temperature})$$

Physically observed : undercooling $(u < 0)$ in liquid and
superheating $(u > 0)$ for solid is possible

Reason: Surface energy effects are neglected in classical model

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Modified condition

$$u = H \quad (\text{Gibbs–Thomson law})$$

H : mean curvature

Issues:

- Interfaces do not stay smooth (e.g. topological changes)
  We need a weak formulation of $u = H$
- $u = H$ describes isotropic surface energy
  In nature: surface energies are anisotropic (leads to crystals)

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Weak formulation of $u = H$:

$$\int_{\Omega_T} \left(\nabla \cdot \xi - \frac{\nabla \chi}{|\nabla \chi|} \cdot D\xi \frac{\nabla \chi}{|\nabla \chi|} \right) d|\nabla \chi(t)| dt = \int_{\Omega_T} \nabla \cdot (u\xi) \chi dx dt$$

for all $\xi \in C^\infty(\Omega_T, \mathbb{R}^n)$ with $\xi \cdot n = 0$

Important analytical results:

Classical solutions :	Chen, Reitich	(1992)
	Radkevich	(1992)
	Escher, Prüss, Simonett	(2003)
	Mucha	(2005)
Weak solutions :	Luckhaus	(1990)
	Röger	(2004)

Idea for the construction of weak solutions (Luckhaus)
Use implicit time discretization

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Idea for the construction of weak solutions (Luckhaus)

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All results are for the isotropic case

Anisotropic energy

Interfacial energy:

$$\mathcal{F}(\Gamma) := \int_\Gamma \gamma(\nu)\, d\mathcal{H}^{n-1}$$ for a hypersurface γ

$\gamma : \mathbb{R}^d \setminus \{0\} \to \mathbb{R}^+$, one-homogeneous, strictly convex, smooth

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First variation

$$\frac{\delta \mathcal{F}}{\delta \Gamma}(\Gamma)(\xi) = \int_\Gamma H_\gamma (\xi \cdot \nu) d\mathcal{H}^{n-1}$$

$$\text{with} \qquad H_\gamma := \nabla_\Gamma \cdot (D\gamma(\nu))$$

where $D\gamma$ is the gradient of γ

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Anisotropic Gibbs–Thomson law

$$u = H_\gamma, \qquad \text{(Gurtin, 1988)}$$

Weak formulation of anisotropic Gibbs–Thomson law

$$\int_\Omega (\operatorname{div}\xi\,\gamma(\nu) - \nu \cdot D\xi\, D\gamma(\nu))\, d|\nabla\chi| = \int_\Omega \operatorname{div}(u\xi)\chi\, dx$$

Weak formulation of anisotropic Gibbs–Thomson law

$$\int_\Omega (\operatorname{div} \xi \gamma(\nu) - \nu \cdot D\xi D\gamma(\nu)) d|\nabla \chi| = \int_\Omega \operatorname{div} (u\xi)\chi dx$$

Question:
How can we define the energy in the BV–context?

Weak formulation of anisotropic Gibbs–Thomson law

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Question:
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Introduce dual function !

$$\gamma^0(q) = \sup_{p\in\mathbb{R}^d\setminus\{0\}} \frac{p\cdot q}{\gamma(p)} \qquad q \in \mathbb{R}^d \setminus \{0\}$$

γ^0 one-homogeneous, strictly convex, smooth

Important identity

$$\mathcal{F}(\Gamma) = \int_\Gamma \gamma(\nu)\, d\mathcal{H}^{n-1} = \sup\left\{ \int_\Omega \chi \,\mathrm{div}\, \varphi \, dx \mid \gamma^{\mathbf{0}}(\varphi) \le \mathbf{1} \right\}$$

see Amar and Bellettini

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Remarks

- Above identity implies lower semi-continuity of $\mathcal{F}$ w.r.t. L^1
- We can show: first variation of $\mathcal{F}$ is given as:

$$\int_\Omega \{div\xi\gamma(\nu) - \nu \cdot D\xi D\gamma(\nu)\} d|\nabla\chi|$$

Idea: Use sup-definition above and approximation arguments.

Visualize surface energy with the help of

Frank diagram: 1-ball of γ

$$\mathcal{F} = \{p \in \mathbb{R}^d \mid \gamma(p) \leq 1\}$$

Wulff shape: 1-ball of γ^0

$$\mathcal{W} = \{q \in \mathbb{R}^d \mid \gamma^0(q) \leq 1\}$$

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Isoperimetric characterization

Wulff shape $\mathcal{W}$ minimizes surface energy among all surfaces that enclose the same volume

Frank diagrams and Wulff shapes for different surface energies.

Cubic anisotropy (left) and hexagonal anisotropy (right).

Main existence result

Theorem: Assumptions:

i) Ω is a bounded C^1–domain

ii) initial data $u_0 \in L^\infty \cap H^{1,2}$, $\chi_0 \in BV(\Omega, \{0,1\})$,

iii) Dirichlet data $u^D \in H^{1,2}(\Omega)$,

iv) r.h.s $f \in L^\infty(\Omega_T)$.

Then there exists

$$\begin{aligned} \chi &\in L^\infty(\Omega_T, \{0,1\}), \ |\nabla \chi(t)| \le C \\ u &\in [u^D + L^2(0,T; H_0^{1,2}(\Omega))] \cap L^\infty(0,T; L^2(\Omega)) \end{aligned}$$

such that

Main existence result (continued)

$$\int_0^T \int_\Omega (u+\chi)\partial_t\varphi + \int_\Omega (u_0+\chi_0)\varphi(0) = \int_0^T \int_\Omega \nabla u \cdot \nabla \varphi - \int_0^T \int_\Omega f\varphi$$

for all $\varphi \in C_0^\infty([0,T)\times\Omega)$, and

$$\int_0^T \int_\Omega (\operatorname{div}\xi D\gamma(\nu)\cdot\nu - \nu\cdot D\xi D\gamma(\nu))\, d|\nabla\chi(t)|dt = \int_{\Omega_T} \operatorname{div}(u\xi)$$

for all $\xi \in C^1(\overline{\Omega}_T, \mathbb{R}^d)$ with $\xi\cdot n = 0$ on $\partial\Omega$.

Proof

As Luckhaus use an implicite time discretization:

$$h > 0 \text{ time step} .$$

Assume $u^h(t-h)$, $\chi^h(t-h)$ is given.
Define functional

$$F_{h,t}(\chi) := \int_\Omega \gamma(\nu) d|\nabla\chi| - \tfrac{1}{2}(u(\chi))^2 - u(\chi)\chi + u(\chi)(u^h(t-h) + \chi^h(t-h))$$

such that

$$(u+\chi) - (u^h(t-h) + \chi^h(t-h)) - h\Delta u = hf^h(t)$$

$$+ \text{ b.c.}$$

$F_{h,t}$ can be interpreted as negative entropy !

$F_{h,t}$ has minimizer $\chi^h(t)$ (use direct method)

Note: γ is convex

Define $u^h(t)$ as a solution of time discrete diffusion equation

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Lemma (energy estimate)

$$\operatorname*{ess\ sup}_{0\le t\le T}\left(\|u^h(t)\|^2_{L^2}+\int_\Omega \gamma(\nu^h)\right)+\int_0^T\int_\Omega |\nabla u^h|^2\le C$$

$$\int_0^T \|\partial_t^{-h}(u^h+\chi^h)(t)\|^2_{H^{-1,2}(\Omega)}\le C$$

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Proof: Test diffusion equation by $u^h - u^D$ and use

$$F_{h,t}(\chi_i^h)\le F_{h,t}(\chi_{i-1}^h)$$

Use standard compactness results and compactness results of Alt and Luckhaus to obtain convergent subsequence of (u^h, χ^h)

Passing to the limit in diffusion equation is standard

Minima of (χ^h, u^h) of $F_{h,t}$ fulfills

$$
\begin{aligned}
0 = &\int_\Omega (\operatorname{div} \xi D\gamma(\nu^h(t)) \cdot \nu^h(t) - \\
&\nu^h(t) \cdot D\xi D\gamma(\nu^h(t)))d|\nabla \chi^h(t)| - \int_\Omega \operatorname{div} (u^h(t)\xi)\chi^h(t) + \\
&\int_\Omega \operatorname{div} (L_h^0(u^h(t) - u^h(t-h) + \chi^h(t) - \chi^h(t-h))\xi)\chi^h(t)
\end{aligned} \tag{1}
$$

for all $\xi \in C^\infty(\overline{\Omega}, \mathbb{R}^d)$, with $\xi \cdot n = 0$, where $\nu^h(t) = -\frac{\nabla \chi^h(t)}{|\nabla \chi^h(t)|}$ where $v = L_h^0(g)$ is the solution of $v - h\Delta v = -g$ in Ω $v = 0$ on $\partial\Omega$

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Goal: Pass to the limit in the discrete Gibbs–Thomson equation (1)

We observe

$$\int_\Omega \gamma(\nu^h) d|\nabla \chi^h| \to \int_\Omega \gamma(\nu) d|\nabla \chi| \quad \text{as} \quad h \to 0$$

Use

- lower semicontinuity of $\int_\Omega \gamma(\nu) d|\nabla \chi|$

and

- strong convergence of u^h in L^2,
- the fact that χ^h solve a minimization problem involving $\int_\Omega \gamma(\nu) d|\nabla \chi|$

Main difficulty: Show $D\gamma(\nu^h) \to D\gamma(\nu)$

[Convergence in the Cahn–Hoffmann ξ–vector]

Since

$$\int_\Omega \gamma(\nu)|\nabla\chi| = \sup\left\{\int_\Omega \chi \,\mathrm{div}\,\varphi dx \mid \varphi \in C^1(\Omega,\mathbb{R}^d),\ \gamma^0(\varphi(x)) \le 1\right\}$$

we obtain a $g_\varepsilon \in C_0^1(\Omega,\mathbb{R}^d)$ with $\gamma^0(g^\varepsilon) \le 1$ such that

$$\int_\Omega (\gamma(\nu) - g_\varepsilon \cdot \nu) d|\nabla\chi| \le \tfrac{1}{3}\varepsilon$$

Claim:

g_ε is a good approximation of the Cahn–Hoffmann vector

$$\xi = D\gamma(\nu)$$

Technical observation

If γ is strictly convex in the sense that
there exists a $d_0 > 0$ such that

$$(D^2\gamma^0)(p)q \cdot q \geq d_0|q|^2 \quad \text{for all} \quad p, q \in \mathbb{R}^n,\ |p| = 1,\ p \cdot q = 0$$

Then we obtain (using a Lemma of Dziuk)
$\exists\, C > 0\ \forall\, \nu \in S^{d-1},\ p \in \mathbb{R}^d$ with $\gamma^0(p) \leq 1$

$$\boxed{C|D\gamma(\nu) - p| \leq \gamma(\nu) - p \cdot \nu}$$

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$$\boxed{C|D\gamma(\nu) - p| \leq \gamma(\nu) - p \cdot \nu}$$

Hence
$\gamma(\nu) - p \cdot \nu$ small implies
p is a good approximation of the ξ–vector $D\gamma(\nu)$

Steps:

$$\int_\Omega (\gamma(\nu) - g_\varepsilon \cdot \nu)) d|\nabla \chi| \leq \tfrac{1}{3}\varepsilon$$

$$\int_\Omega \gamma(\nu^h) d|\nabla \chi^h| \to \int_\Omega \gamma(\nu) d|\nabla \chi|$$

implies

g_ε is a good approximation of $D\gamma(\nu)$ and $D\gamma(\nu^h)$

This can be used to show

$$\int_\Omega \nu^h \cdot D\xi D\gamma(\nu^h) d|\nabla \chi^h| \to \int_\Omega \nu \cdot D\xi D\gamma(\nu) d|\nabla \chi|$$

Convergence in the other terms of the weak formulation is easier (and omitted here)
We finally obtain the weak formulation

$$\int_0^T \int_\Omega (\operatorname{div} \xi D\gamma(\nu) \cdot \nu - \nu \cdot D\xi(\nu) D\gamma(\nu)) d|\nabla \chi| = \int_{\Omega_T} \operatorname{div}(u\xi)\chi$$

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Related result by Rybka (1999):

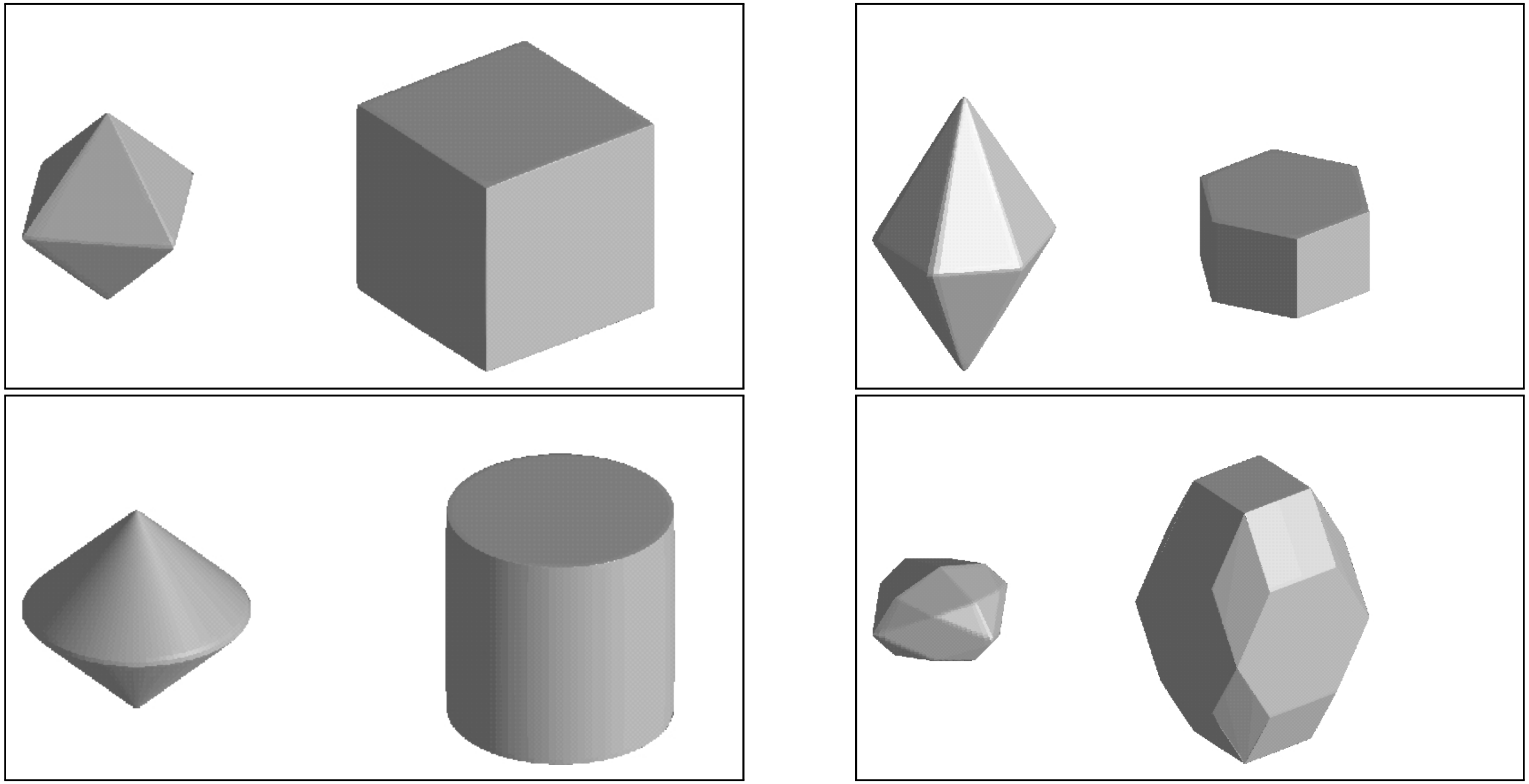
- space dimension 2,
- crystalline curvature,
- no facet braking allowed.

Numerical solutions

Stefan problem with kinetic undercooling

$$\begin{array}{rcll}
\partial_t u - \Delta u & = & f & \text{in liquid and solid} \\
\left[\frac{\partial u}{\partial \nu}\right] & = & -\frac{1}{\mathcal{S}}\mathcal{V} & \text{Stefan condition on interface } \Gamma \\
\frac{1}{\beta(\nu)}\mathcal{V} & = & H_\gamma - \mathcal{S}u & \text{generalized Gibbs–Thomson relation} \\
 & [.] & & \text{jump across interface} \\
 & \mathcal{S} & & \text{undercooling} \\
 & \beta & & \text{kinetic coefficient}
\end{array}$$

We can handle e.g. the following anisotropies



Frank diagrams (left) and Wulff shapes (right)

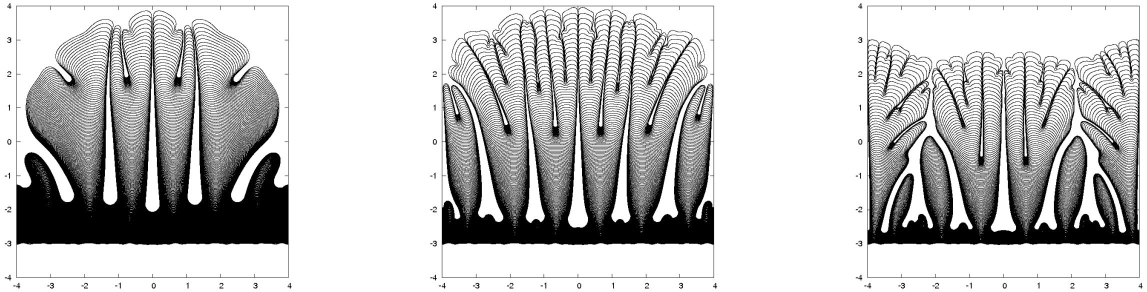
Stability

Continuous Lyapunov structure (u_D constant)

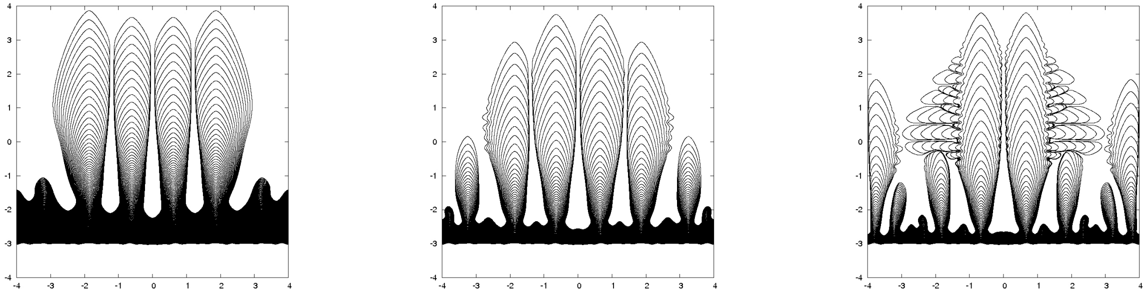
$$\frac{d}{dt}\left(\int_\Omega (u-u_D)^2 + \mathcal{F}(\Gamma) + u_D vol(\Omega_s(t))\right) + \int_\Omega |\nabla u|^2 + \int_\Omega \frac{\mathcal{V}^2}{\beta(\vec{\nu})} ds \le (f, u-u_D)$$

We obtain a discrete analogue of the above inequality even in the anisotropic case

Mullins Sekerka instability in 2D



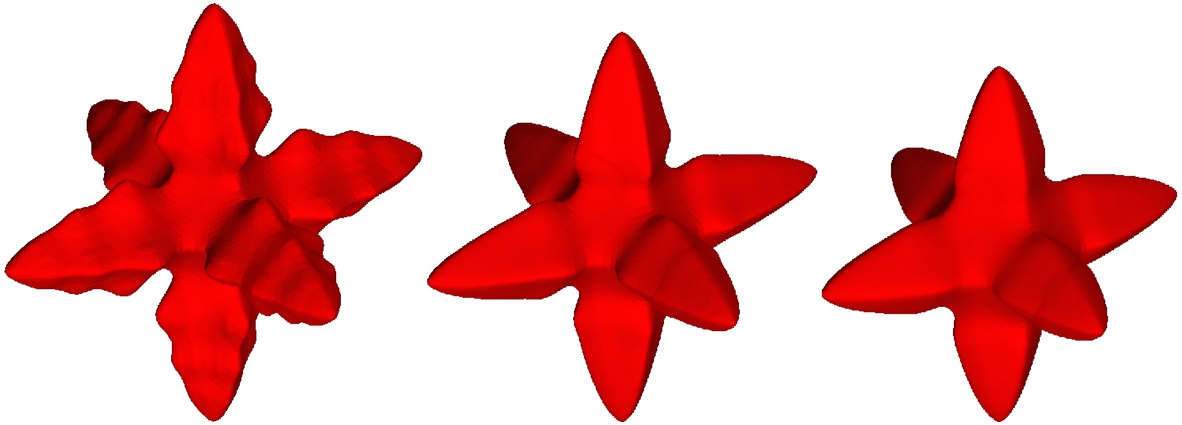
undercooling $\mathcal{S} = 1$, isotropic surface energy 5×10^{-3}, 2×10^{-3}, 10^{-3}



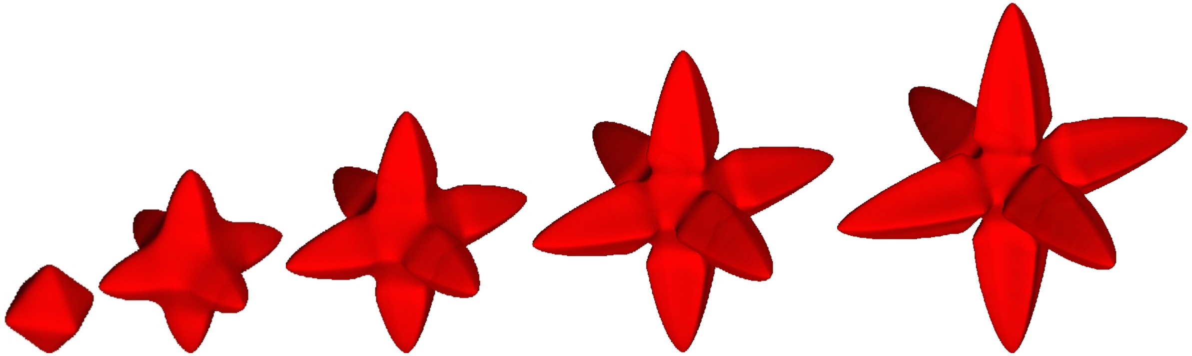
undercooling $\mathcal{S} = 1$, cubic anisotropy with prefactor 5×10^{-3}, 2×10^{-3}, 10^{-3}

Solidification with cubic anisotropy

- Small sphere as initial data



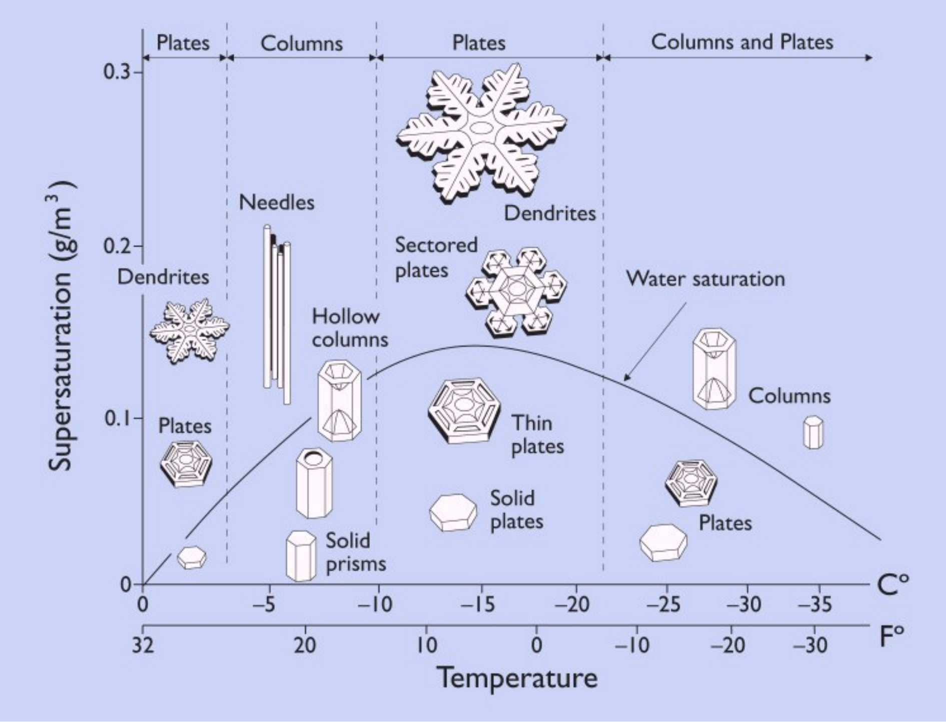
- Computation for different refinements. Oscillations disappear for fine grids

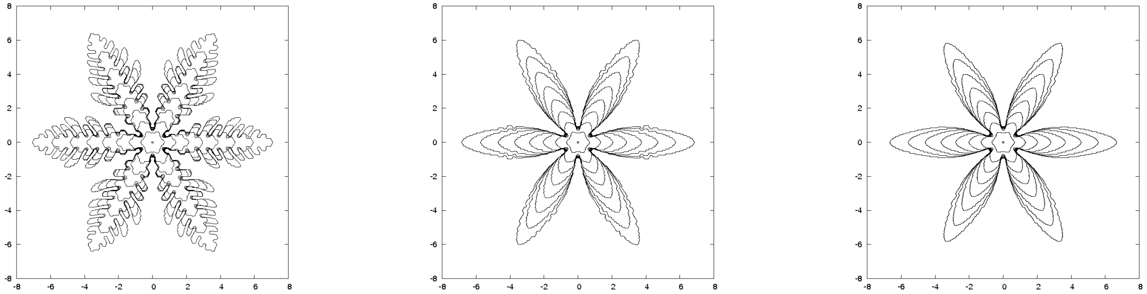


Details of the evolution on finest grid

Hexagonal symmetry (snow crystal symmetry)

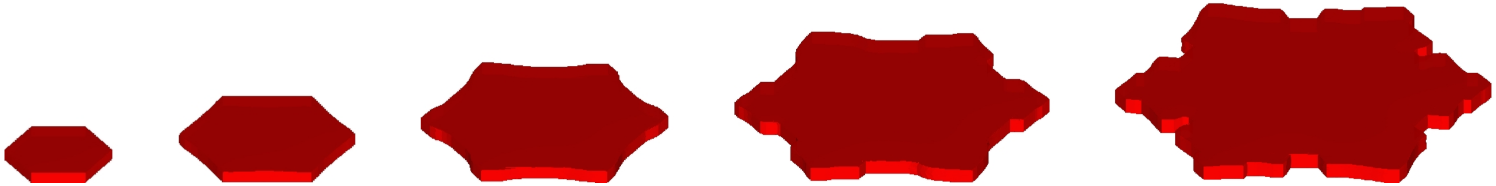
Morphology diagram of Nakaya



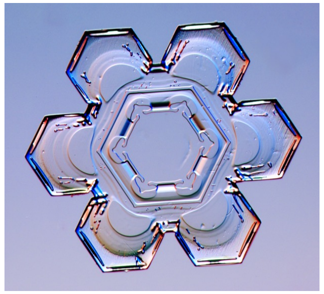


2D-computation

Classical snow crystals

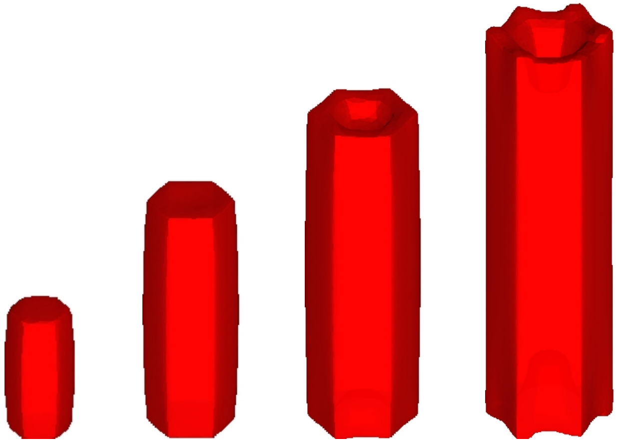


formation of plates



real snowflake

Many forms need 3D computations

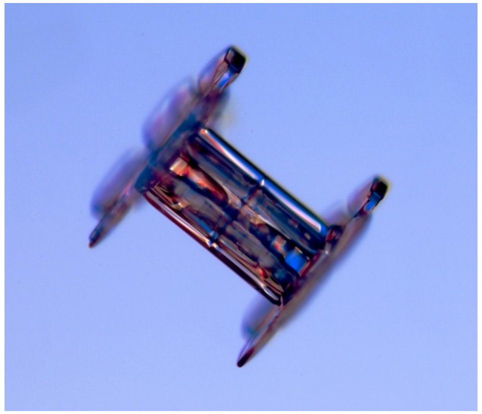


Formation of hollow columns (facet braking)

Compare analytical results by Giga and Rybka (2008)

real snowflake

Another 3D effect



A more pronounced real snowflake

Remarks and Conclusions

- We showed global existence of weak solutions for the Stefan problem with anisotropic Gibbs-Thomson law
- The general crystalline case is still open
- We introduced stable finite element discretization with good mesh properties (No redistancing of mesh points necessary)
- Hence: crystalline anisotropies can be approximated in a stable and efficient way
- The Stefan problem with anisotropic Gibbs-Thomson law models realistic crystal growth phenomena