Efficient computation of crystal growth using sharp interface methods

Harald Garcke

University of Regensburg

joint with John Barrett (London)
Robert Nürnberg (London)

July 2010

Outline

1. Curvature driven interface motion
2. Numerical methods for geometric flows
3. The new approach
4. Anisotropy
5. Stefan problem

Curvature driven interface motion

Issue:

Compute the motion of hypersurfaces where the normal velocity is given in terms of curvature

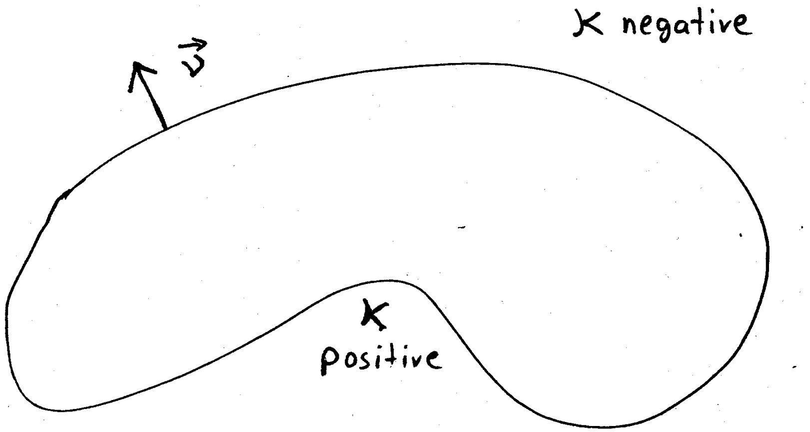
Applications:

Materials science	(grain growth, solidification)
Epitaxial growth	(surface diffusion)
elastic flows	(Willmore flow, elastic rods, biological membranes)
general relativity	(positive mass theorem)
computer graphics	(image and surface processing)

Curvature driven interface motion

Notation

$\Gamma = (\Gamma_t)_{t\in[0,T]}$	evolving surface	$\vec{\nu}$	unit normal
$\mathcal{V}$	normal velocity	H	mean curvature



$\vec{H} = H\vec{\nu}$ mean curvature vector Δ_s surface Laplacian

Curvature driven interface motion

Examples of geometric flows

$\mathcal{V} = H$	mean curvature flow
$\mathcal{V} = f(H)$	e.g. $\mathcal{V} = -\frac{1}{H}$ inverse mean curvature flow
$\mathcal{V} = -\Delta_s H$	surface diffusion
$\mathcal{V} = -\Delta_s H - H\lvert\nabla_s \nu\rvert^2 + \frac{1}{2}H^3$	Willmore flow (elastic flow)
$+$	anisotropic versions
$+$	coupling to bulk quantities

Curvature driven interface motion

Properties of the flows

1.) Surface area decreasing

$$\frac{d}{dt} \int_{\Gamma_t} 1 \, d\mathcal{H}^{d-1} \leq 0$$

O.K. for mean curvature flow, surface diffusion

2.) Volume preserving

$$\frac{d}{dt} \text{ volume } = \int_{\Gamma_t} \mathcal{V} \, d\mathcal{H}^{d-1} = - \int_{\Gamma_t} \Delta_s H \, d\mathcal{H}^{d-1} = 0$$

Gauß theorem!

O.K. for surface diffusion

Numerical methods for geometric flows

Numerical methods for mean curvature flow I

$\mathcal{V} = H$

Approaches	:	Level set methods	(Osher, Sethian, ...)
		Phase field method	(Caginalp, Elliott, ...)
		Graphs	
In this talk	:	Parametric approach	

Numerical methods for mean curvature flow II

Use parametrisation

$$(\rho, t) \mapsto \vec{x}(\rho, t) \in \mathbb{R}^d$$

$$\rho \in M, \quad M \text{ reference manifold}$$

$$t \in [0, T]$$

We compute normal velocity as $\mathcal{V} = \vec{x}_t \cdot \vec{\nu}$

Problem: How do we compute mean curvature?

Use parametric approach

Dziuk for the first time discretized

$$\Delta_s \vec{x} = H\,\vec{\nu}$$

with piecewise linear continuous finite elements
and solves a discrete version of

$$\vec{x}_t = \Delta_s \vec{x} \qquad (= H\,\vec{\nu})$$

to approximate mean curvature flow
Not necessary: Original equation only prescribes normal velocity.

Numerical methods for geometric flows

Review of Results

Many analytical and computational results are known for this approach:

- stability is known
- error estimates ($d = 2$, Dziuk, Deckelnick)
- computations for dendritic growth possible (Schmidt)
- anisotropy can be included (Dziuk, Deckelnick)

Disadvantages

- no generalization to $\mathcal{V} = f(H)$ possible
- generalization to fourth order flows is difficult
- mesh distortions possible

A new approach for curvature driven flows

Idea: Work with two variables $(\vec{X}, H)$ and write the flow as:

$$\mathcal{V} = \vec{X}_t \cdot \vec{\nu} = H \ , \quad H\vec{\nu} = \Delta_s \vec{X} \ .$$

A new approach for curvature driven flows

Idea: Work with two variables $(\vec{X}, H)$ and write the flow as:

$$\mathcal{V} = \vec{X}_t \cdot \vec{\nu} = H \,, \quad H\vec{\nu} = \Delta_s \vec{X} \,.$$

Numerical discretization:

time steps : $0 = t_0 < t_1 < \cdots < t_{n-1} < t_n = T$,
$\tau_m := t_{m+1} - t_m$

polyhedral surface : $\Gamma^m = \bigcup$ simplices

FE spaces : W_m^h piecewise linear cont. FE over Γ^m

$V_m^h = [W_m^h]^d$

Discrete version of the weak formulation:

Solve the discrete version of the weak formulation:

$$\begin{aligned}
\left\langle \frac{\vec{X}^{m+1}-\vec{X}^{m}}{\tau_m}, \chi \vec{\nu}^{m} \right\rangle_m^h - \langle H^{m+1}, \chi \rangle_m^h &= 0 & \forall\, \chi \in W_m^h \\
\langle H^{m+1} \vec{\nu}^{m}, \vec{\eta} \rangle_m^h + \langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \rangle_m &= 0 & \forall\, \vec{\eta} \in V_m^h
\end{aligned}$$

Here $\langle ., . \rangle_m$ and $\langle ., . \rangle_m^h$ are inner products over Γ^m (using mass lumping).
Evaluate ∇_s using the “old” metric.

How does the mesh behave ?

For $d = 2$ we obtain for the semi-discrete version:

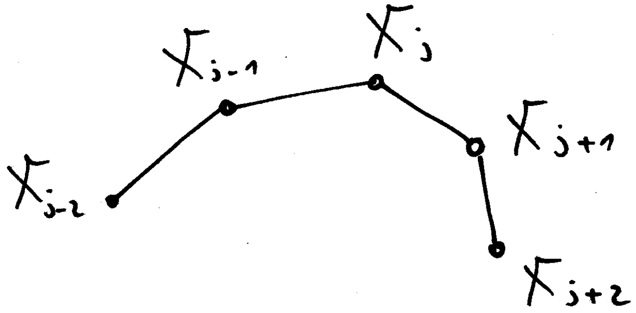
Either

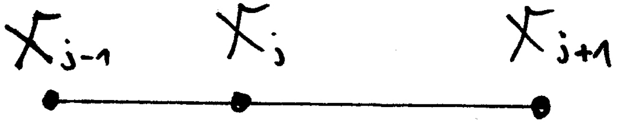
$$|\vec{X}_{j+1} - \vec{X}_j| = |\vec{X}_j - \vec{X}_{j-1}|$$

or

$$(\vec{X}_{j+1} - \vec{X}_j) \| (\vec{X}_j - \vec{X}_{j-1})$$

Idea of proof: Test with a suitable approximation of the tangent.



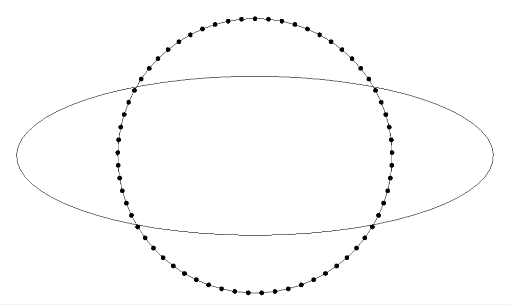


Numerical methods for geometric flows

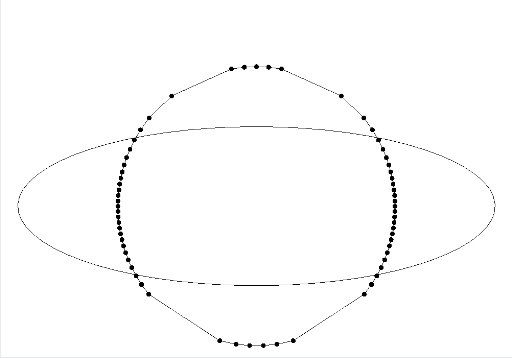
Implications for the fully discrete scheme

Tendency for equidistribution of mesh points !

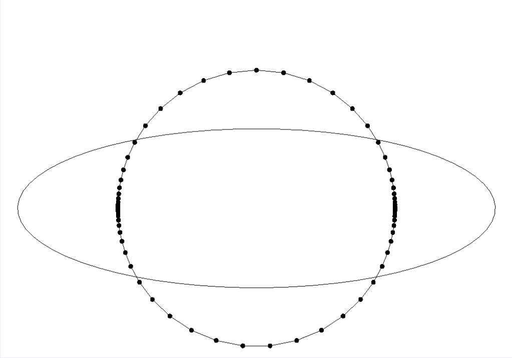
Examples for surface diffusion



Our scheme



Dziuk scheme



Bänsch Morin Nochetto scheme

Schemes of Dziuk and Bänsch, Morin, Nochetto work well after mesh redistribution !

Our algorithm can be rewritten as:

Find $\vec{X}^{m+1}$ as a solution of (neglect numerical integration)

$$\underbrace{\int_{\Gamma^m} |\nabla_s \vec{X}|^2}_{\text{Dirichlet integral}} + \underbrace{\frac{1}{\tau_m}\int_{\Gamma^m}((\vec{X} - \vec{X}^m)\cdot\vec{\nu}^m)^2 \quad \to \quad \text{min}}_{\substack{\text{small to higher order}\\ \text{for tangential variations}}}$$

Our algorithm can be rewritten as:

Find $\vec{X}^{\,m+1}$ as a solution of (neglect numerical integration)

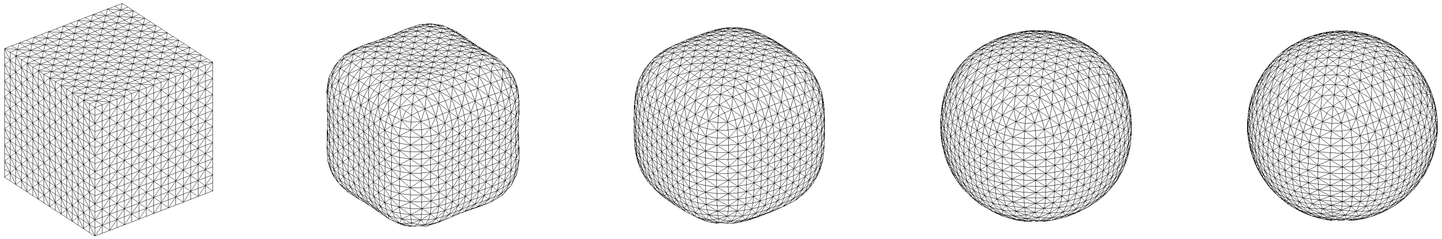
$$\underbrace{\int_{\Gamma^m} |\nabla_s \vec{X}|^2}_{\text{Dirichlet integral}} + \underbrace{\frac{1}{\tau_m}\int_{\Gamma^m} ((\vec{X} - \vec{X}^{\,m}) \cdot \vec{\nu}^{\,m})^2 \quad \rightarrow \quad \text{min}}_{\text{small to higher order for tangential variations}}$$

Theory of minimal surfaces:

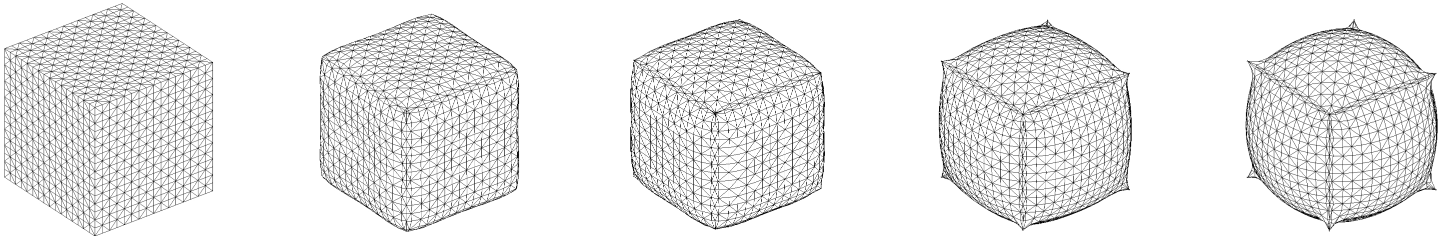
Minimizing the Dirichlet integral under all possible reparametrizations gives a conformal mapping
Here: Discrete conformal mapping (cp. Pinkall + Polthier)

Higher dimensional case

Surface diffusion in 3-d



Our scheme

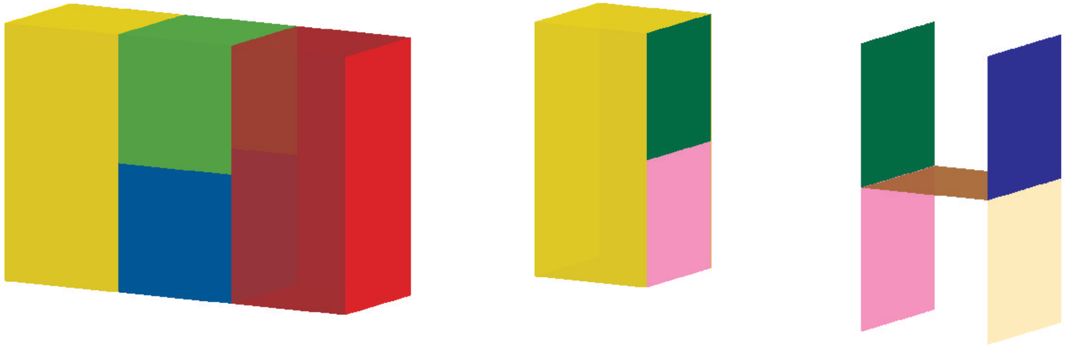


Bänsch, Morin, Nochetto scheme (allowing only velocities in normal direction - similar as Dziuk)

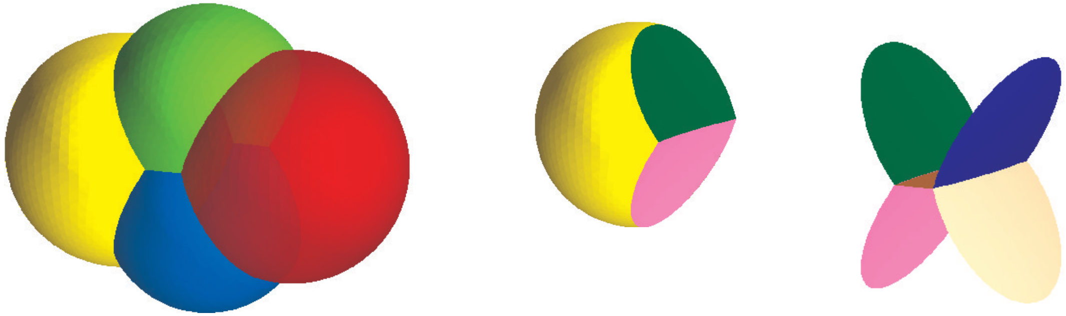
Mesh distortion appears

Triple junction lines

Surface diffusion with triple lines



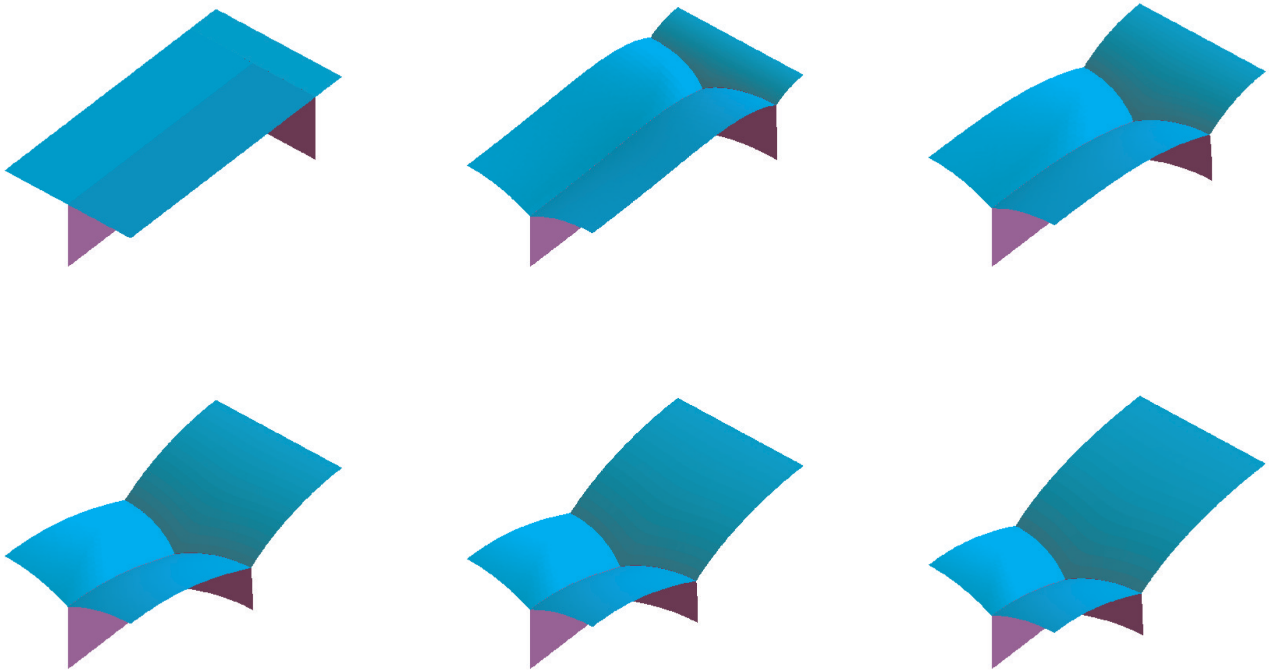
Initial time



Solution at a large time

Coupled Surface diffusion and grain boundary motion

Surface grooves with grain boundaries



Time evolution

How to handle the anisotropy ?

This was a problem in earlier approaches

Problem:	Equations are highly nonlinear It is difficult to obtain stable discretizations
Idea:	Use Riemannian structure as much as possible
Central idea so far:	Discretize

$$H\,\vec{\nu} = \Delta_s \vec{id}$$

Now:	Replace standard Euclidean inner product on $\mathbb{R}^d$ by a (space independent) product

$$(\vec{u}, \vec{v})_{\tilde{G}} = \vec{u} \cdot \tilde{G}\,\vec{v}$$

Ansatz

Define

$$\begin{aligned} \gamma(\vec{\nu}) &= \text{surface element related to } \vec{\nu}^{\perp} \\ &= \det(\vec{\tau}_i \cdot \tilde{G}\vec{\tau}_j)_{i,j=1}^{d-1} \end{aligned}$$

$$\tau_1, \ldots, \tau_{d-1} \quad \text{ONB} \quad \text{of} \quad \vec{\nu}^{\perp}$$

$\rightsquigarrow$ ellipsoidal Wulff shapes

Generalize to ℓ^r-norms of such expressions

$$\gamma(\vec{p}) = \left(\sum_{\ell=1}^{L} [\gamma_\ell(\vec{p})]^r \right)^{\frac{1}{r}},$$

$\gamma_\ell(\vec{p})$ defined as above with the help of $\tilde{G}_\ell$

Do the geometric analysis with respect to the new metric (cf. Bellettini + Paolini) to obtain first variation of

$$\mathcal{F}(\Gamma) = \int_\Gamma \gamma(\vec{\nu})$$

We obtain

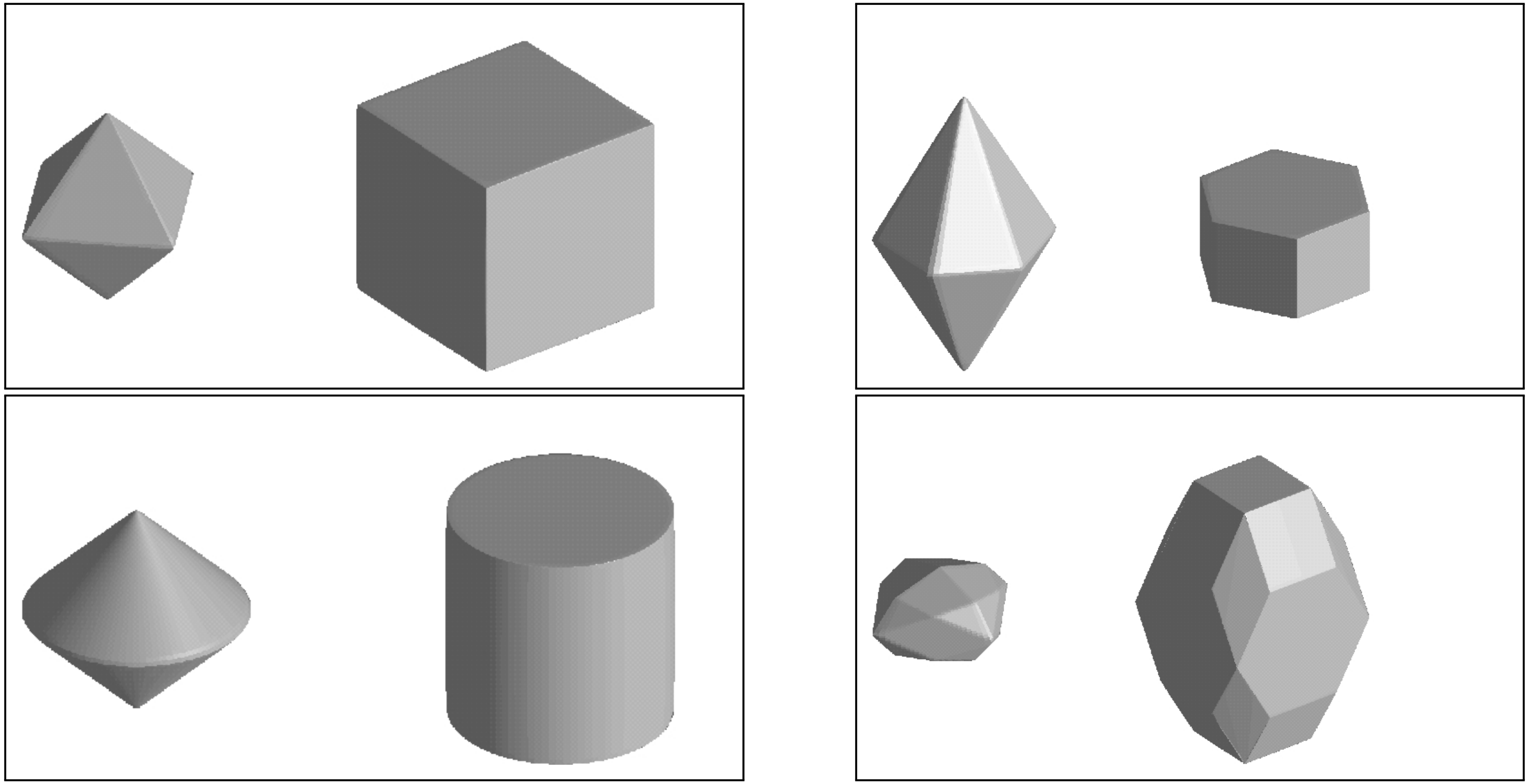
$$H_\gamma \, \vec{\nu} = \sum_{\ell=1}^{L} \gamma_\ell(\vec{\nu}) \, \widetilde{G}_\ell \, \nabla_s^{\widetilde{G}_\ell} \,.\, \left[\left[\frac{\gamma_\ell(\vec{\nu})}{\gamma(\vec{\nu})} \right]^{r-1} \nabla_s^{\widetilde{G}_\ell} \, \vec{\mathrm{id}} \right].$$

$$\int_\Gamma H_\gamma \, \vec{\nu} \,.\, \vec{\varphi} \; d\mathcal{H}^{d-1} =$$

$$-\sum_{\ell=1}^{L} \int_\Gamma \left[\frac{\gamma_\ell(\vec{\nu})}{\gamma(\vec{\nu})} \right]^{r-1} (\nabla_s^{\widetilde{G}_\ell} \, \vec{\mathrm{id}}, \nabla_s^{\widetilde{G}_\ell} \, \vec{\varphi})_{\widetilde{G}_\ell} \, \gamma_\ell(\vec{\nu}) \; d\mathcal{H}^{d-1},$$

$\leadsto$ Weak formulation possible

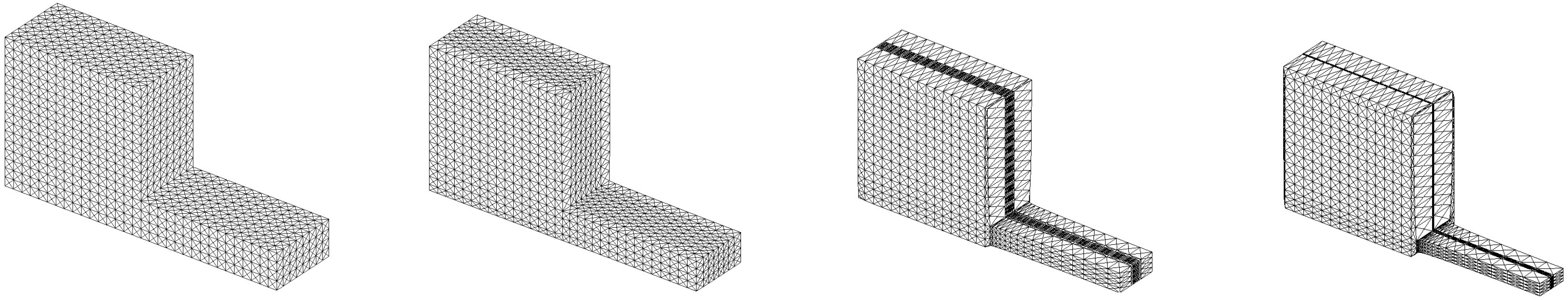
We can handle e.g. the following anisotropies



Frank diagrams (left) and Wulff shapes (right)

Anisotropic geometric evolution equations

Compute facet breaking for crystalline flows

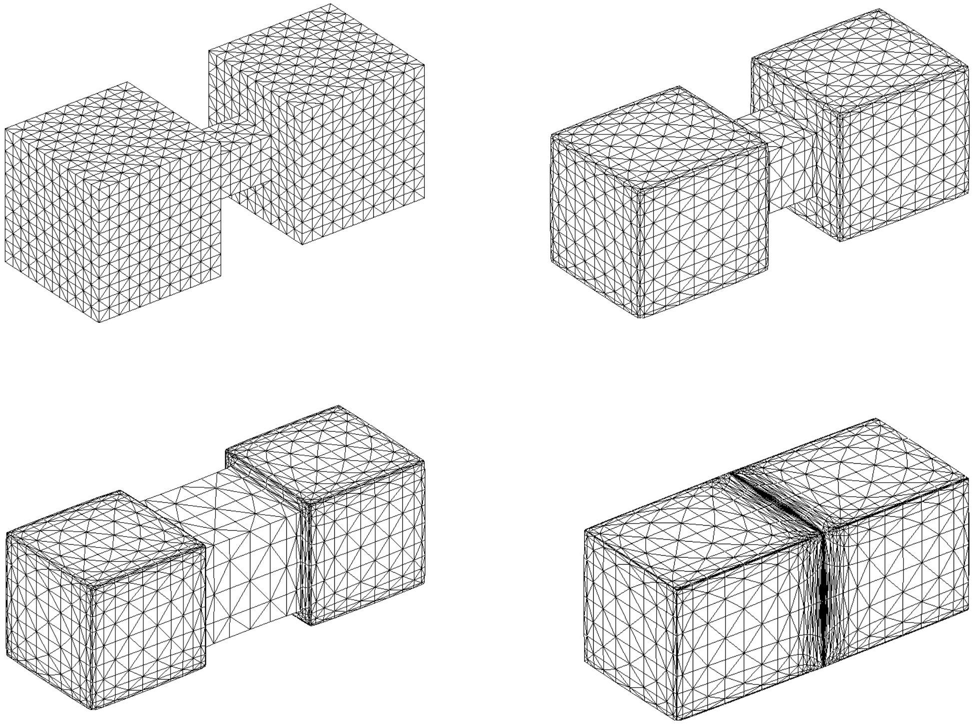


$\vec{X}(t)$ at times $t = 0,\ 0.1,\ 0.2,\ 0.25$

crystalline curvature flow
(facet breaking, cf. Bellettini, Novaga, Paolini)

Anisotropic geometric evolution equations

crystalline surface diffusion

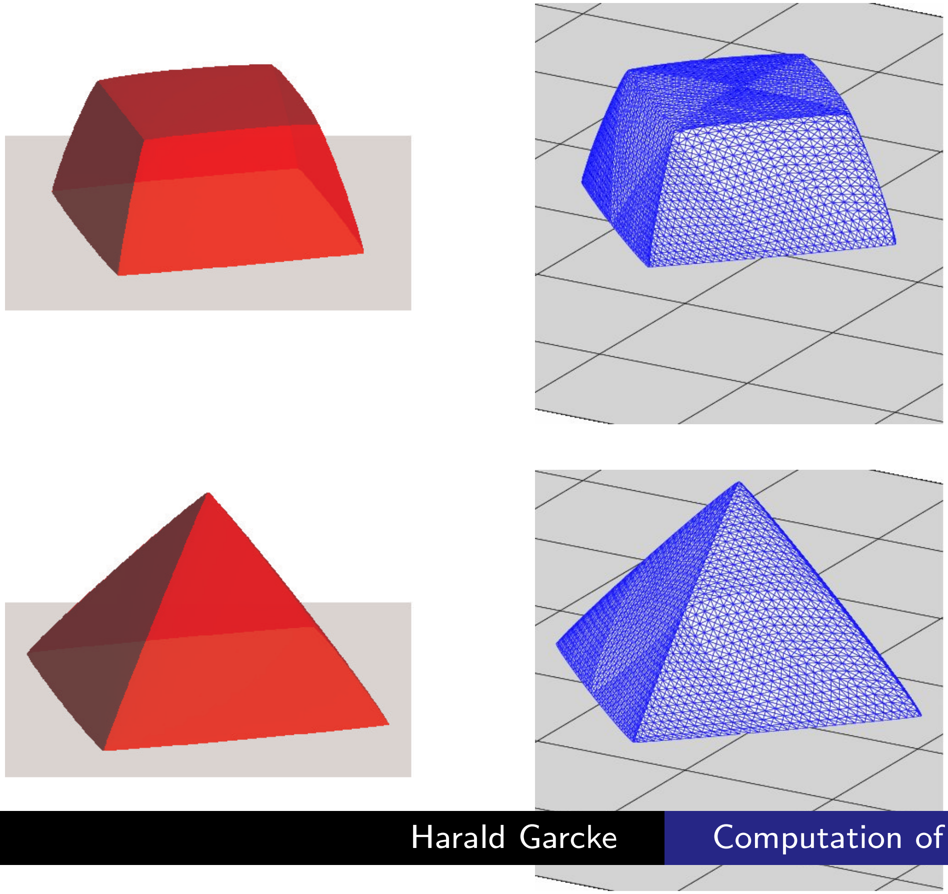


Contact with exterior boundary

Anisotropic surface diffusion with boundary conditions

Initial data: Spherical cap.

Solutions at large times for different anisotropies



Numerical approximation

Stefan problem with kinetic undercooling

$\partial_t u - \Delta u = f$	in liquid and solid
$[\frac{\partial u}{\partial \nu}] = -\frac{1}{\mathcal{S}}\mathcal{V}$	Stefan condition on interface Γ
$\frac{1}{\beta(\nu)}\mathcal{V} = H_\gamma - \mathcal{S}u$	generalized Gibbs–Thomson relation
$[.]$	jump across interface
$\mathcal{S}$	undercooling
β	kinetic coefficient

How to approximate the Stefan problem numerically ?

Approaches so far: A. Schmidt (1993), R. Almgren(1993), ...
Needed: Weak formulation of the Stefan problem

$$(\partial_t u, \phi)_{L^2} + (\nabla u, \nabla \phi) = \int_{\Gamma(t)} (x_t \cdot \nu) \phi \, d\mathcal{H}^{d-1}$$

$$\int_{\Gamma(t)} \frac{x_t \cdot \nu}{\beta(\nu)} \chi \, d\mathcal{H}^{d-1} = \int_{\Gamma(t)} [H_\gamma - u] \chi \, d\mathcal{H}^{d-1}$$

$$\int_{\Gamma(t)} H_\gamma \nu \cdot \eta \, d\mathcal{H}^{d+1} + \int_{\Gamma(t)} \nabla_s x \cdot \nabla_s \eta = 0$$

for suitable test functions

Approximate

Γ	by polyhedral surfaces
u	by a bulk FE function
x	vector FE–function on a reference polyhedron
H	scalar function on reference polyhedron

Stability

Continuous Lyapunov structure (u_D constant)

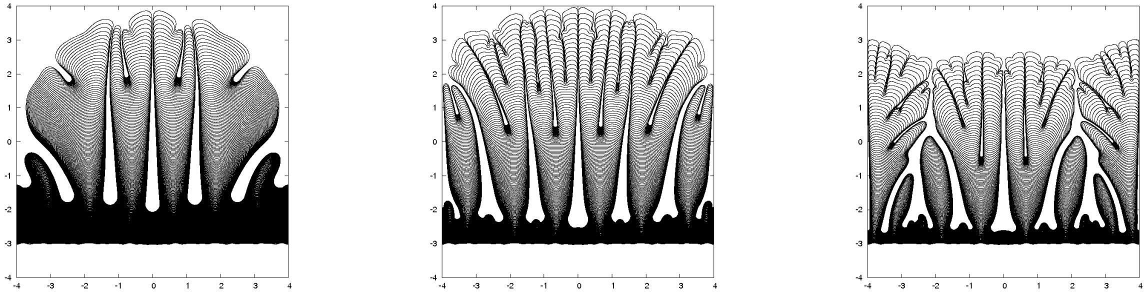
$$\frac{d}{dt}\left(\int_\Omega (u-u_D)^2 + \mathcal{F}(\Gamma) + u_D vol(\Omega_s(t))\right) + \int_\Omega |\nabla u|^2 + \int_\Omega \frac{\mathcal{V}^2}{\beta(\vec{\nu})} ds \leq (f, u-u_D)$$

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

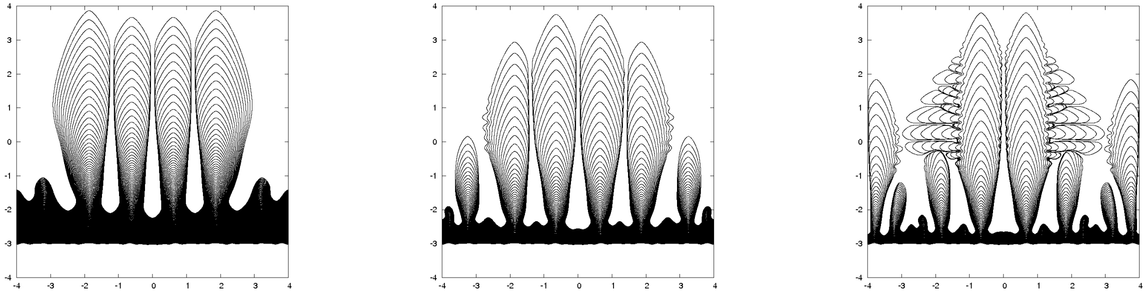
Proof:

- Testing procedure
- Generalize a Lemma of Bänsch to estimate surface energy

Mullins Sekerka instability in 2D



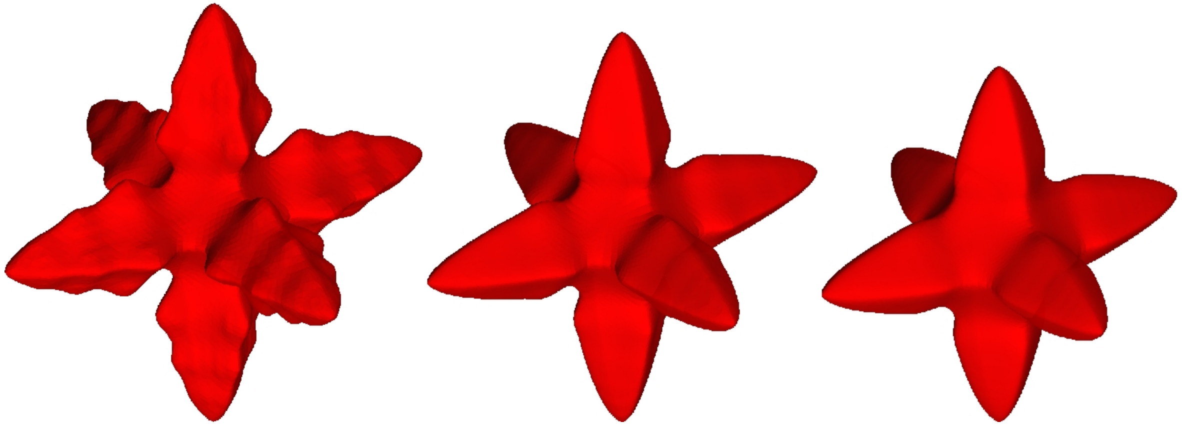
undercooling $\mathcal{S} = 1$, isotropic surface energy 5×10^{-3}, 2×10^{-3}, 10^{-3}



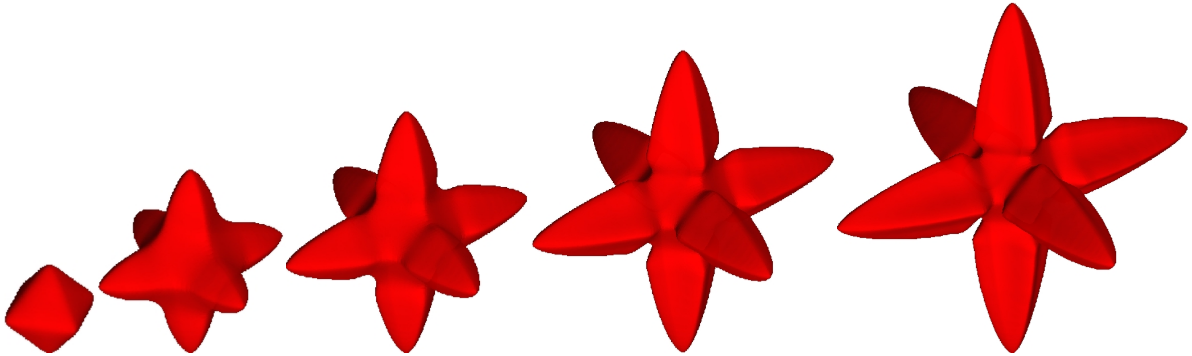
undercooling $\mathcal{S} = 1$, cubic anisotropy with prefactor 5×10^{-3}, 2×10^{-3}, 10^{-3}

Solidification with cubic anisotropy

- Small sphere as initial data



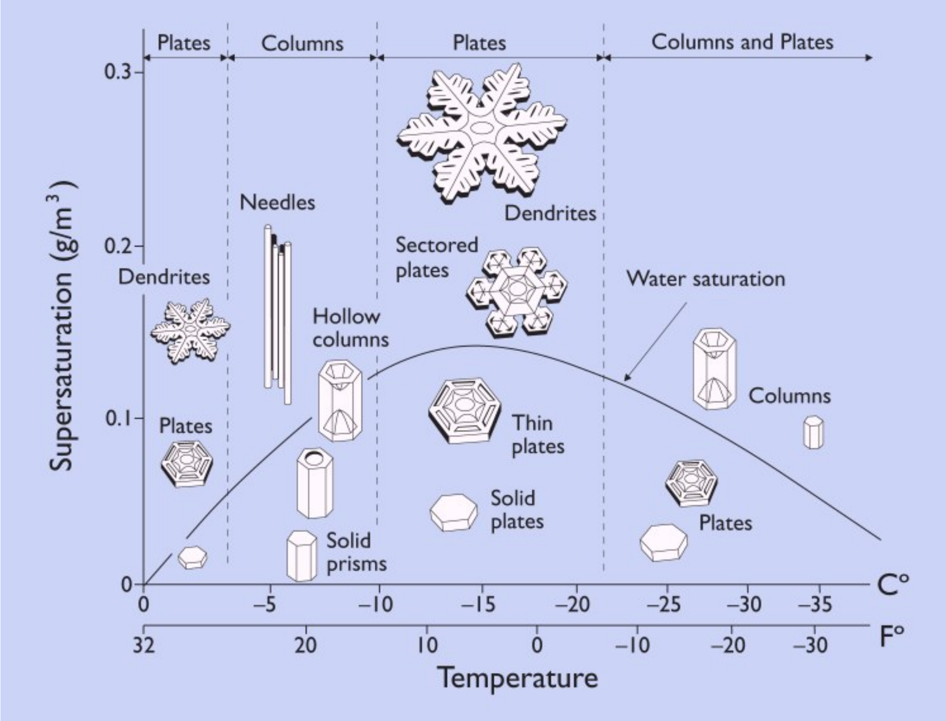
- Computation for different refinements. Oscillations disappear for fine grids

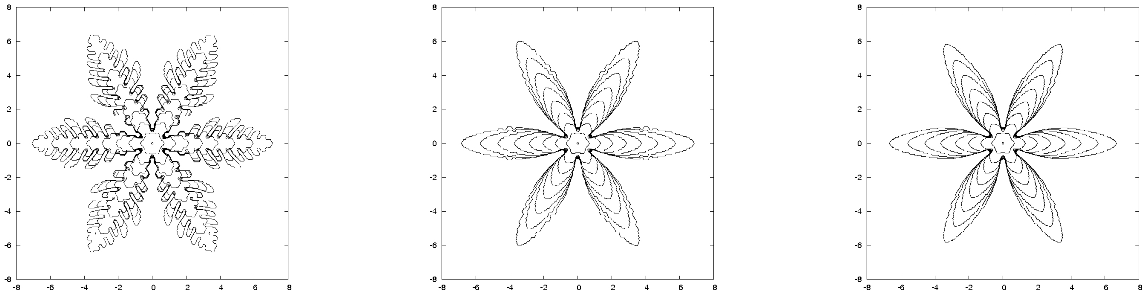


Details of the evolution on finest grid

Hexagonal symmetry (snow crystal symmetry)

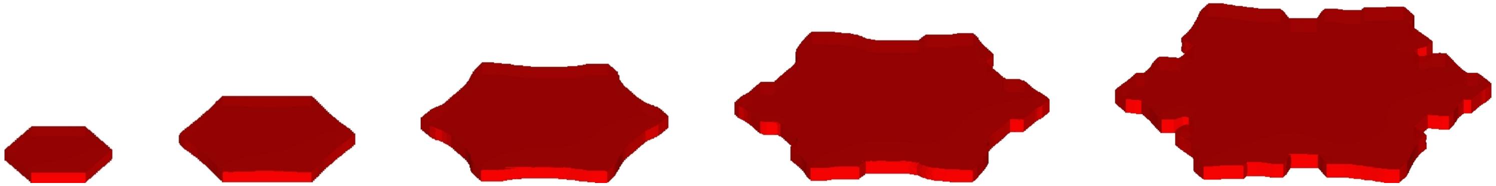
Morphology diagram of Nakaya



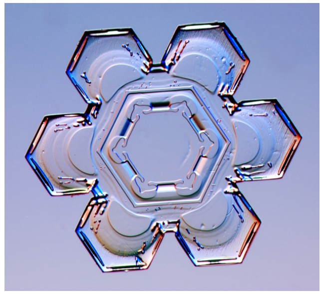


2D-computation

Classical snow crystals

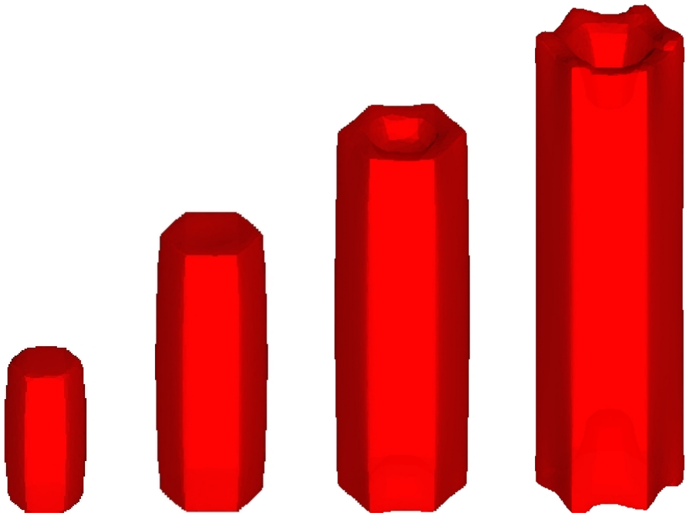


formation of plates



real snowflake (photo due to K. Libbrecht)

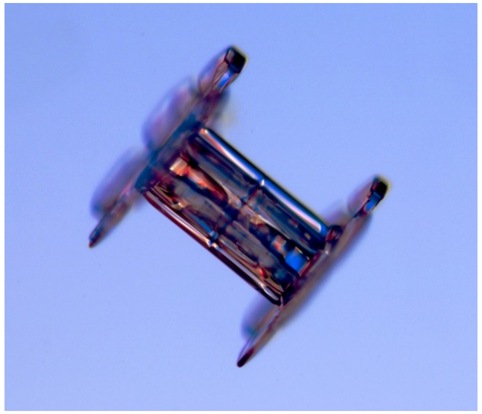
Many forms need 3D computations



Formation of hollow columns (facet braking)

real snowflake

Another 3D effect



A more pronounced real snowflake

Remarks and Conclusions

- We derived stable finite element discretization with good mesh properties
  (No redistancing of mesh points necessary)
- Crystalline anisotropies can be approximated in a stable and efficient way
- Method is applicable and efficient also for quasi-static variants (Mullins–Sekerka problem)

$$\begin{aligned} \partial_t u - \Delta u = 0 \quad &\rightsquigarrow \quad -\Delta u = 0 \\ \frac{1}{\beta(\nu)}\mathcal{V} + u = H_\gamma \quad &\rightsquigarrow \quad u = H_\gamma \end{aligned}$$