Very singular diffusion equations: second and fourth order models for crystal growth phenomena

– On some macroscopic PDE models for crystal growth –

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June 2012

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1. Introduction / Macroscopic PDE models for an evolving crystal surface including facets

1.1 Nearly flat crystal surface (below roughening temperature)

1.2 A single crystal growth with facets

Singular diffusion equations
= Fast diffusion equations

(i) $u_t = (|u_x|^{p-2} u_x)_x \quad 1 < p < 2$ (singular)

(ii) $u_t = (\mathrm{sgn}\, u_x)_x \qquad p = 1$ (very singular)

If we write in the form of $u_t = a(u_x) u_{xx}$,

(i) $\Leftrightarrow a(r) = (p-2)|r|^{p-2}$ $\left[a(r) \to \infty \text{ as } r \to 0, a \in L^1_{loc}\right]$.

(ii) $\Leftrightarrow a(r) = 2\delta(r)$ $\left[a \notin L^1_{loc}\right]$.

If $\int_{-1}^{1} a(r) dr = \infty$, then patterns instantaneously disappear.

e.g. equation for the inverse function $u = u(x,t)$ of $x = x(u,t)$ satisfying the heat eq $x_t = x_{uu}$

L. C. Evans (1996), Y. G. Chen – K. Sato – Y. Giga (1997)

1. Macroscopic PDE models with facet

1.1 Nearly flat crystal surface

(phenomena below roughening temperature)

- $h = h(x,t)$: height of a crystal

  at $x \in \mathbf{R}^n$ and $t \geq 0$

- Free energy (often proposed)

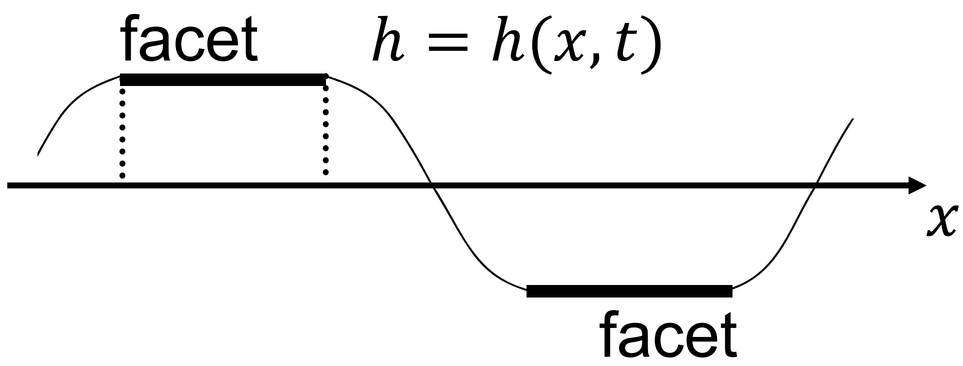
$$E(h) = \int_{\mathbf{T}^n} \left(|\nabla h| + \frac{q}{3} |\nabla h|^3 \right) dx, \quad q > 0$$

$\mathbf{T}^n$: periodic cell

H. Spohn (1993), J. Phys. I. France

(I) Evaporation model

$$h_t = -\frac{\delta E}{\delta h}$$



or

$$h_t = \mathrm{div}\left(\frac{\nabla h}{|\nabla h|}\right) + q\,\mathrm{div}(|\nabla h|^2 \nabla h)$$

one dimensional version

$$h_t = (\mathrm{sgn}\, h_x)_x + q(|h_x|^2 h_x)_x$$

If $q = 0$, it is the total variation flow.
(Used for image denoising.)

(II) Relaxation model
(motion by surface diffusion)

H^{-1} gradient flow of E

$$h_t = \Delta \frac{\delta E}{\delta h}$$

or

$$h_t = -\Delta \left[\operatorname{div}\left(\frac{\nabla h}{|\nabla h|} \right) + q \operatorname{div}(|\nabla h|^2 \nabla h) \right], q > 0$$

If $q = 0$, the system is a 4-th order total variation flow.

1.2 A single crystal growth (with facets)

- Stefan problem with Gibbs – Thomson effect and kinetic supercooling
- One phase
- Quasi-static approximation
- Both interfacial energy and kinetic coefficient is anisotropic (depending on orientation of crystal surface)

Unknowns

$\Omega(t)$: a bounded domain in $\mathbf{R}^n$ occupied by a crystal at time $t \geq 0$

$\sigma = \sigma(x,t)$: supersaturation at x outside a crystal $(\mathbf{R}^n \setminus \overline{\Omega}(t))$

Given functions

$\gamma_0 : S^{n-1} \to (0,\infty)$ surface energy density

$\gamma(p) := |p|\gamma_0(p/|p|)$ homogeneous extension of γ_0 in $\mathbf{R}^n$

$M : S^{n-1} \to (0,\infty)$ mobility

$1/M$: kinetic coefficient

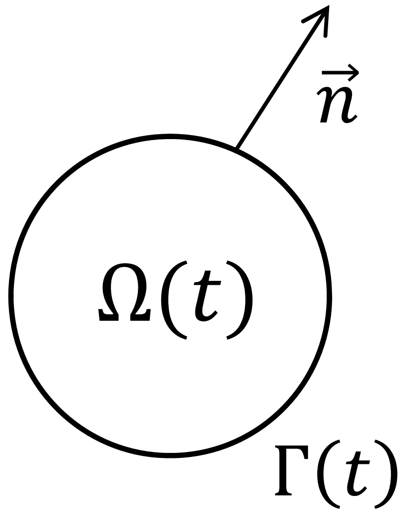
Notations and concepts

$\Gamma(t) := \partial\Omega(t)$ crystal surface in $\mathbf{R}^n$

$\vec{n}$: outer unit normal of $\Gamma(t)$

$\kappa_\gamma := -\mathrm{div}_\Gamma\left(\nabla_p \gamma(\vec{n})\right)$ anisotropic mean curvature

V : normal velocity in the direction of $\vec{n}$



Equations

$$\begin{cases} -\Delta\sigma = 0 \text{ in } \mathbf{R}^n \setminus \overline{\Omega(t)} \\ \dfrac{\partial\sigma}{\partial\vec{n}} = V \text{ on } \Gamma(t) \text{ (Stefan condition)} \\ \boxed{V = M(\vec{n})\left(\kappa_\gamma + \sigma\right) \text{ on } \Gamma(t)} \end{cases}$$

(curvature flow equation with driving force term)

(cf. Y. G. Surface Evolution Equations, 2006)

$(\sigma, \Omega(t))$ unknown!

- If $\gamma_0 = 1$, then interfacial energy is isotropic and κ_γ is nothing but an usual ($(n-1)$ times) mean curvature.
- The mobility M can be anisotropic.

Equilibrium shape ($\sigma = \mathrm{const}$)

- Wulff shape

$$W_{\gamma_0} = \bigcap_{|m|=1} \{x \mid x \cdot m \le \gamma_0(m)\}$$

is a substitute of ball for anisotropic case.
Indeed, formally

$$\kappa_{\gamma_0} = -(n-1) \text{ on } \partial W_{\gamma_0}$$

(For smooth strictly convex energy,
$\kappa_{\gamma_0} = \mathrm{const} \Rightarrow \Gamma = \partial W_{\gamma_0}$ (Alexandrov type result))

- If γ_0 is smooth and strictly convex in the sense that Frank $\gamma = \{ p \mid \gamma(p) \leq 1\}$ has positive principle curvatures, this problem is locally well-posed for a given initial data $\Omega(0)$ and condition at space infinity or boundary condition at a ball containing $\Omega(0)$. (e.g. C. M. Elliott – K. Deckelnick ’99 but two-phase) (one-phase, Hele – Shaw, isotropic, 2-D P. Mucha, ’06)

- Recent simulation for snow crystal (with singular γ) : (J. Barrett – H. Garcke – R. Nürnberg ’11).

Our situation

Frank γ is still convex but may have a corner (so that W_{γ_0} has a flat part.)

Typical example: If Frank γ is a polytope, γ_0 is called crystalline.

Why we say very singular?

The main reason is that the singularity is so strong in the equation so that its evolution speed is a nonlocal quantity. We shall see this property by simple examples. Note that the meaning of a solution is either nontrivial or unknown.

2. Core examples
(curvature flow with driving force)

(a) $u_t = (\operatorname{sgn} u_x)_x + \sigma(x), x \in \mathbf{R}, t > 0$

More generally,

(b) $u_t = a(u_x)\left[\left(W'(u_x)\right)_x + \sigma(x)\right]$

W: convex, may not C^1

$a \neq \text{const} \Rightarrow$ non−divergence type

[Note: σ is given]

Feature

Energy density W has jump discontinuities so that diffusion is singular.

(a) is of the form

$$u_t = 2\delta(u_x)u_{xx} + \sigma(x).$$

Simple examples

(a) with $\sigma = 0$: total variation flow

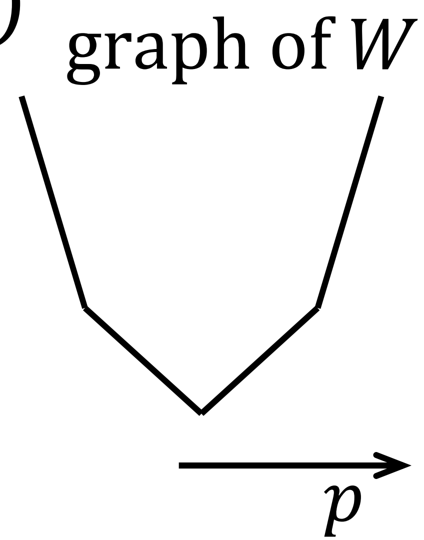
(b) with crystalline W

: crystalline curvature flow for a graph−like function $y = u(x,t)$

$W(p)$: piecewise linear, convex (crystalline)

$a(p) = (1 + |p|^2)^{1/2}$, $\sigma =$ constant

S.B. Angenent – M. Gurtin '89, J. Taylor '91



Fourth order examples

(c) $u_t = -\Delta \left[\mathrm{div} \left(\frac{\nabla u}{|\nabla u|} \right) \right]$

4th order total variation flow

(d) $u_t = -\Delta \left[\mathrm{div} \left(\frac{\nabla u}{|\nabla u|} \right) + q \, \mathrm{div}(|\nabla u|^2 \nabla u) \right]$

relaxation dynamics

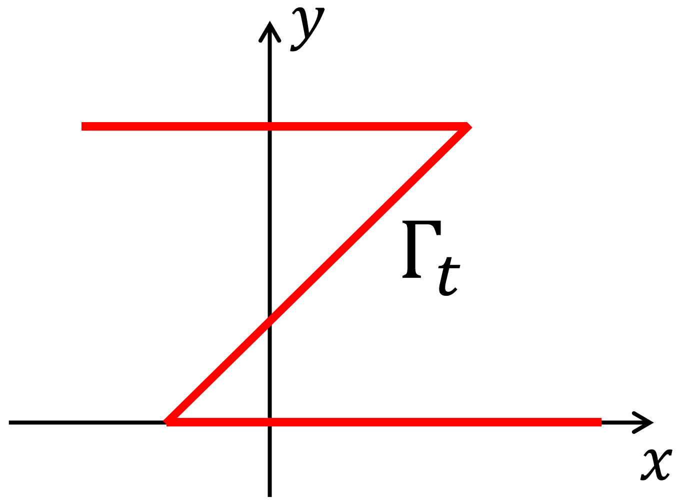
Further example (second order) (Vertical Diffusion)

Burgers eq. $u_t + uu_x = 0$

$\Leftrightarrow V = y$ on $\Gamma_t \qquad (*)$

$\Gamma_t = \{(x,y);\ y = u(x,t)\}$

(graph of u)



A solution of $(*)$ may overturn and cannot be viewed as the graph of an entropy solution.

Consider

$$V = y - M\,\mathrm{div}\nabla_p \gamma(\vec{n}), \quad \gamma(p_1, p_2) = |p_2|$$

Instead of $(*)$, where $M > 0$.

Thm (M.-H. Giga – Y. G. ’03)

If $M > 0$ is sufficiently large (with respect to jump size), then overturn is prevented and Γ_t becomes the graph of an entropy solution at least for the Riemann problem.

cf. Y. G. ’02, Y.-H. R. Tsai – Y.G. – Osher ’02, Y. Brenier: ’09 formulation by an obstacle functional

Other examples

- Kobayashi – Warren – Carter model for averaged angle of multi-grain motion

  (K. Shirakawa's talk) (R. Kobayashi – J. Warren – C. Carter '00)

- 1-harmonic map flow

  $u_t = \mathrm{div}\left(\frac{\nabla u}{|\nabla u|}\right) + |\nabla u|u\,,\quad u : S^2$-valued

  (Denoising chromaticity of images)

  Y. G. – H. Kuroda '04; Y. G. – Y. Kashima, N. Yamazaki, '04; … L. Giacomelli – S. Moll '10

Notion of Solutions

(1) Subdifferential formulation (a) (not (b)), (c), (d)

$u_t \in -\partial E(u)$ T. Fukui − Y. G.'96 ($a = \mathrm{const}$ (a))

σ : general

(c), (d) Y. Kashima '03, '12

(2) Viscosity approach : (b)

M.-H. Giga − Y. G. '98, '99, '01

σ : const, $u_t + F(u_x, (W'(u_x))_x + \sigma) = 0$

M.-H. Giga − Y. G. − P. Rybka '11

σ : nonconstant : comparison principle

(3) Variational approach for distance functions

G. Bellettini et al. '01～

3. Speed of facets and finite time extinction

3.1 Characterization of the speed

3.2 Evaluating nonlocal quantity

3.3 Finite time extinction

3.1 Characterization of the speed

Consider simplest eq $(W(p) = |p|, \sigma \equiv 0)$

$$u_t = (\operatorname{sgn} u_x)_x.$$

What is the speed of the facet (flat part)?

Assume 'facet stays as facet'

$$\int_{a-\delta}^{b+\delta} u_t = W'(-\bar{\delta}) - W'(+\tilde{\delta})$$

$$\Leftrightarrow u_t = \frac{-2}{b-a} \quad (\delta \downarrow 0)$$

$$\tilde{\delta} = u_x(a-\delta), -\bar{\delta} = u_x(b+\delta)$$

⟶ Crystalline flow for admissible polygon.

Speed of Evolution

Thm (Kōmura, Brezis - Pazy)

H: Hilbert space, E: convex, lower semicontinuous, $u_0 \in H$

⇒ There exists a **unique** solution $u \in C([0,\infty),H) \cap AC([\delta,T],H)$ solving

$$\frac{du}{dt} \in -\partial E(u) \quad \text{a.e.} \quad t > 0, \; u(0) = u_0.$$

Moreover, u is right differentiable for all $t > 0$ and

$$\frac{d^+u}{dt} = -\partial^0 E(u).$$

canonical restriction / minimal section:

$$-\partial^0 E(u) = \operatorname{argmin}\{\|f\|_H \,;\, f \in \partial E(u)\}$$

Solution knows how to evolve!

3.2 Evaluating nonlocal quantity

What is the quantity

$\Lambda_W^\sigma = (W'(u_x))_x + \sigma(x)$ **?**

In general Λ_W^σ **is not constant on the facet so that facet may break.**

How to calculate the Speed

$$E(u) = \int_{\mathbf{T}} \{W(u_x) - \sigma(x)u\}\,\mathrm{d}x\,, \mathbf{T} = \mathbf{R}/\mathbf{Z}\,, H = L^2(\mathbf{T}),$$

$$f \in \partial E(u) \Leftrightarrow f = -\eta_x - \sigma, \eta(x) \in \partial W(u_x(x)),$$

$$f^0 = \partial^0 E(u)$$

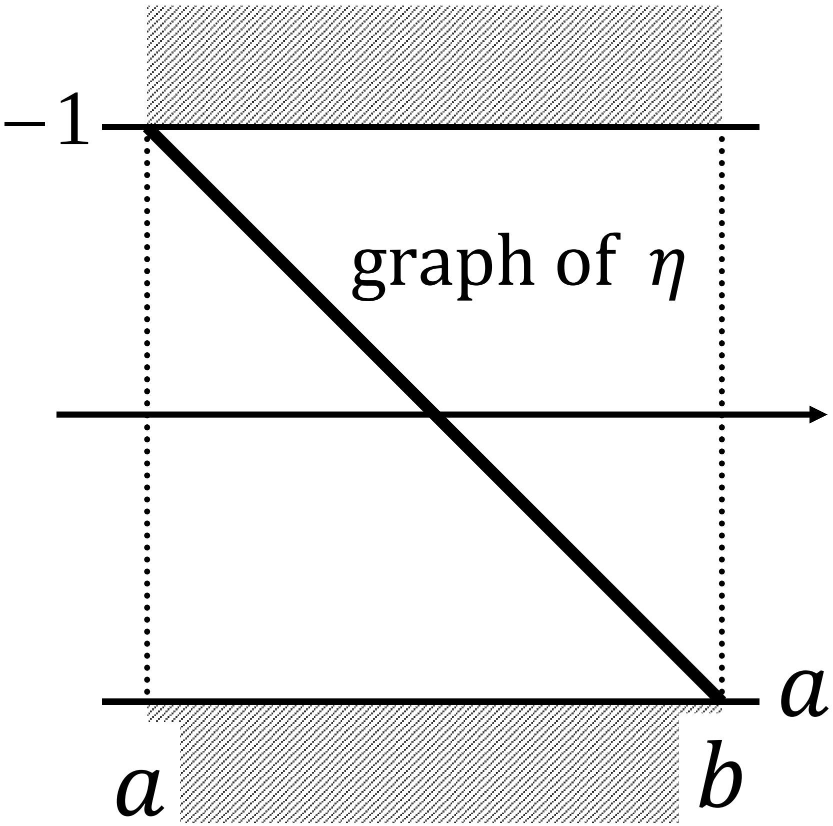
$$\Leftrightarrow f^0 = \mathrm{argmin}\left\{ \int_{\mathbf{T}} |f|^2 \mathrm{d}x; f = -\eta_x - \sigma, \eta(x) \in \partial W(u_x(x)) \right\}.$$

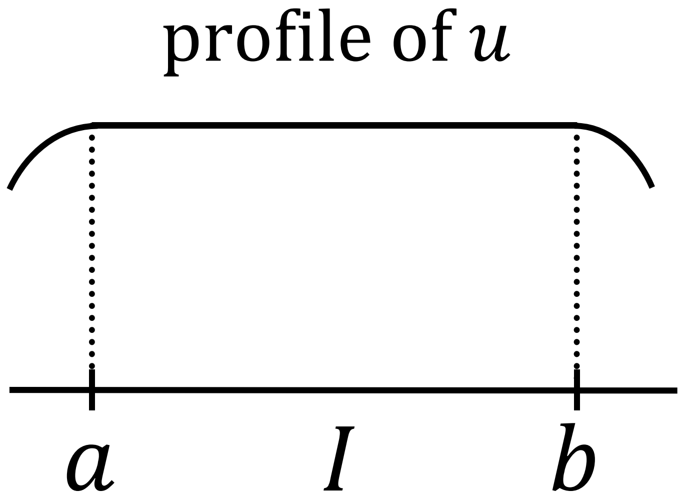
Obstacle type condition at the place where the slope belongs to the jump of W.

Formally, $\Lambda_W^\sigma = -f^0$.

Values of Λ_W^σ

The case $\sigma = \mathrm{const}$





$$\Lambda_W^\sigma(u) = -\frac{2}{b-a} + \sigma$$

Higher dimensional case ($\sigma = 0$)

$$E(u) = \int_{\mathbf{T}^n} |\nabla u| \mathrm{d}x$$

Even if one considers a facet F (with slope zero) of a concave function,

' $\Lambda = \mathrm{div}\left(\frac{\nabla u}{|\nabla u|}\right)$ ' may not be a constant.

'Find z such that

$$\begin{cases} \mathrm{div}\, z = \mathrm{const} & \text{on} \quad F \\ |z| \leq 1 & \text{on} \quad F \\ z \cdot \nu = 1 & \text{on} \quad \partial F \end{cases}$$'

If such z exists, then $\Lambda = \mathrm{const}$ (calibrable).

Definition: If F admits a solution of this problem, F is called a Cheeger set.

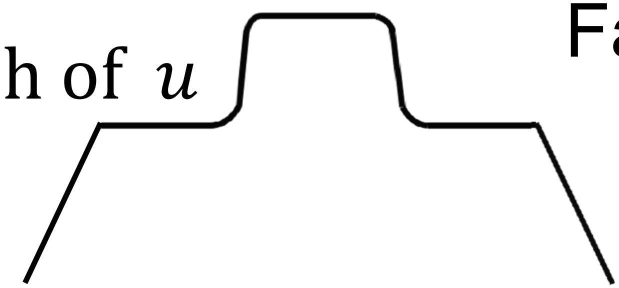
G. Bellettini – M. Novaga – M. Paolini '99: Counterexample of constancy of Λ

Bellettini, Novaga, Paolini '01 $\Lambda \in L^{\infty}$ and BV, sufficient condition for a Cheeger set

Kawohl, Lachand - Robert '06: Characterization of Cheeger set

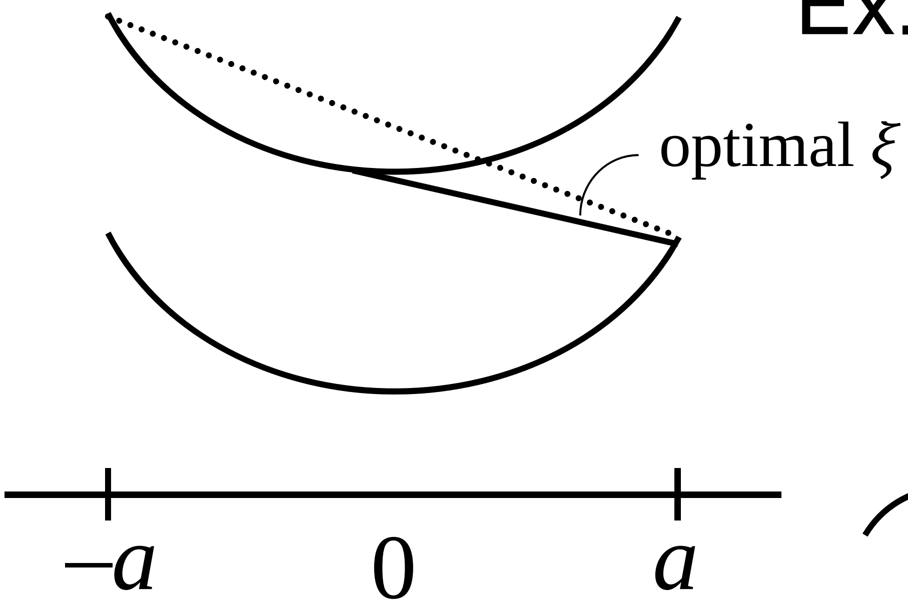
- Little is known for a Cheeger set except for a convex facet on concave function

graph of u



Facet : annulus $\Rightarrow \Lambda = \mathrm{const}$

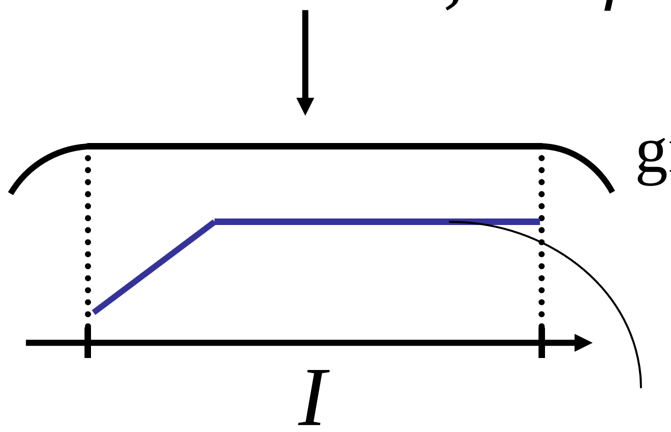
Obstacle Problem



Ex. $\sigma(x) = 2x,\ I = (-a, a)$

a : not small

$$\xi := \eta + \int \sigma$$



$\xi' =$ const. on I

$\Leftrightarrow I$ is calibrable (Cheeger set)

Note: Two part of Λ_W^σ cannot split

Some explicit Solutions

(1) σ : const **Angenent – Gurtin, Taylor**

'admissible polygon'

(2) $\sigma(x) = \sigma(-x), \sigma_x > 0, \text{e.g. } a(p) = (1+p^2)^{1/2}$

Explicit solution starting with $u_0 \equiv 0$.

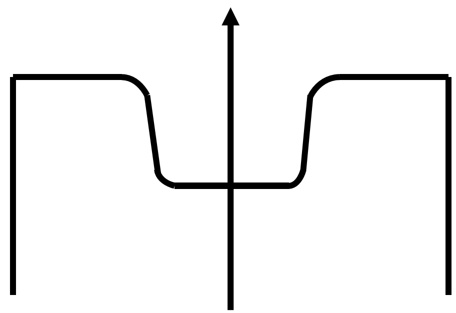
(bending solution)

Nonlocal Hamilton-Jacobi equations with unusual free boundary

Y.G. – Gorka – Rybka (2010)

Y.G. – Rybka (2009)

[M.-H. Giga – Y.G. '98 for (a)]

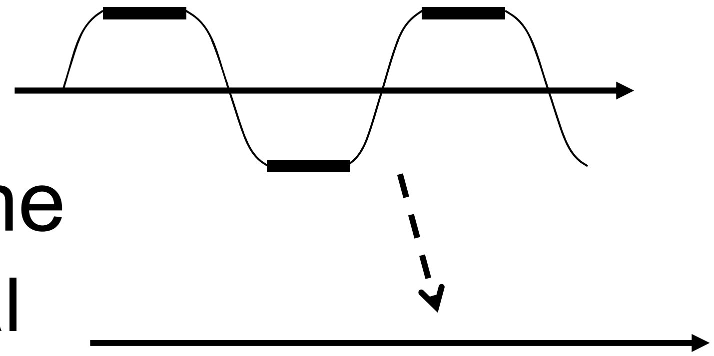


3.3 Finite time extinction

Does a pattern remain or not?

- Second order problem for total variation one can compare typical solutions (see e.g. a book of Andreu, Caselles, Mazon '04)
- Fourth order problem for total variation or even relaxation dynamics

Neverthless, one obtain an estimate for the extinction time T^* from above by a norm of initial data. We impose periodic BC.



Thm (R. V. Kohn – Y. G. ’11)

Consider relaxation model or 4-th order total variation flow under periodic BC. Assume that the space dimension $n \leq 4$. Then the extinction time is estimated as

$$T^*(u_0) \leq C\left\|(-\Delta)^{-1}u_0 \colon \dot{W}^{-1,p}\right\|^{(1/\theta)-1} \cdot \|u_0 \colon H^{-1}\|^{2-1/\theta},$$

where u_0 is the initial data. Here C is a scale-in dependent constant and $1 + n/2 = \theta(n-1) + (1-\theta)(3+n/p),\ 1 \leq p < \infty,\ 1/2 < \theta \leq 1.$

Open for $n \geq 5$. For $n = 4$, the proof is easy. Multiply $(-\Delta)^{-1}u$ with the equation and integrate by parts yields $\frac{1}{2}\frac{d}{dt}\|u\|_{H^{-1}}^{2} = -\int|\nabla u|$. Use Calderon – Zygmund and Sobolev inequilities to estimate RHS from above by $-\|u\|_{H^{-1}}$ when $n = 4$. In general we use interpolation inequilities as well as growth estimate for negative norm.

4. Well-posedness
(second order problem)

Viscosity theory is so far well-established for a curve evolution when $\sigma = \text{constant}$ even if Frank γ has corners.

Thm (M.-H. Giga – Y. G. '01)

For a given initial data E_0 (compact set in R^2) there is a unique global level-set flow $\{E(t)\}_{t\geq 0}$ for

$$V = M(\vec{n})\left(\kappa_\gamma + \sigma\right)$$

provided that σ is constant in x and $M > 0$ is continuous. (More general dependence on κ_γ is allowed)

(Here Frank γ is convex and may have corners outside the corners the curvature is assumed to be bounded)

Level-set flow for smooth γ : Y.-G. Chen – Y. G. – S. Goto '91 L. C. Evans – J. Spruck '91; see also a book of Y. G. (2006)

Thm (M.-H. Giga – Y. G. '01) (Approximation)

Assume that $\gamma_\varepsilon \to \gamma$, $M_\varepsilon \to M$ uniformly. Assume that $E_0^\varepsilon \to E_0$ in Hausdorff distance sense. Then the level set solutions E^ε converge to E in the sense

$$\sup_{0<t<T} d_H(E^\varepsilon(t), E(t)) \to 0 \ \text{ as } \ \varepsilon \to 0$$

provided that E is regular up to T, i.e. $E(t) = \overline{D(t)}$ (for $t \in (0,T]$) where $D(t)$ is a flow starting from $D_0 = \operatorname{int} E_0$.

- Similar theorems are expected to be true for non constant σ but so far only comparison principle for a graph-like function is established. (M.-H. Giga – Y. G. – P. Rybka '11)

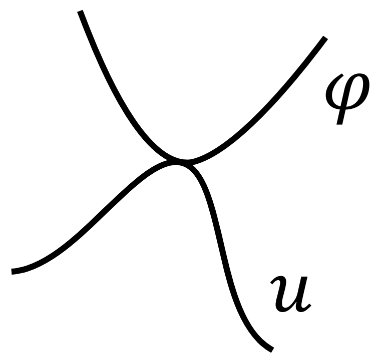
Rough idea of notion of solutions

Viscosity approach

Classical case. We say u is a subsolution of $u_t - a(u_x)u_{xx} = 0$ $(a \geq 0)$ if

$$\varphi_t - a(\varphi_x)\varphi_{xx} \leq 0 \text{ at } (\hat{x},\ \hat{t})$$

whenever $u - \varphi$ takes its maximum in $Q = \mathbf{R} \times (0, \infty)$ at $(\hat{x},\ \hat{t})$ for $\varphi \in C^\infty(Q)$.



Our case (b) : $u_t - a(u_x)\Lambda_W^\sigma(u) = 0$

- Choice of test function φ
- Assign nonlocal quantity

$$\Lambda_W^\sigma(u) = (W'(u_x))_x + \sigma(x)$$

on the facet

Higher dimension: Existence and comparison principle with no σ (M.-H. Giga, Y. G., N. Pozar, in preparation '12)

Variational approach
(Bellettini – Novaga – Paolini '01～)

$$V = \gamma \kappa_\gamma \text{ for } \Gamma(t) \subset \mathbf{R}^n (n \geq 2)$$

The anisotropic signed distance function $\mathrm{d}(x, \Gamma)$ (unit ball is the Wulff shape of γ) is required to fullfill

$$d_t - \mathrm{div} \nabla \gamma(\nabla d) \geq 0 \text{ in a nbd of } \Gamma(t)$$
$$= 0 \text{ on } \Gamma(t)$$

Underlining idea

$$V = \kappa$$

$$d = d(x, \Gamma) \text{ fulfills } d_t - \Delta d \geq 0 \text{ in } \mathbf{R}^n$$

Comparison principle is OK / Existence is just for convex case

(G. Bellettini, V. Caselles, A. Chambolle, M. Novaga '06)

5. Effect of kinetic and interfacial anisotropy

In what way a beautiful hexagonal snow flakes appear?

Conventional physical explanation

$$V = M(\vec{n})(\kappa + \sigma), \quad M(\vec{n}) \geq 0$$

The kinetic coefficient dominates the growth shape since κ is negligible. Then, the equation looks like HJ equation

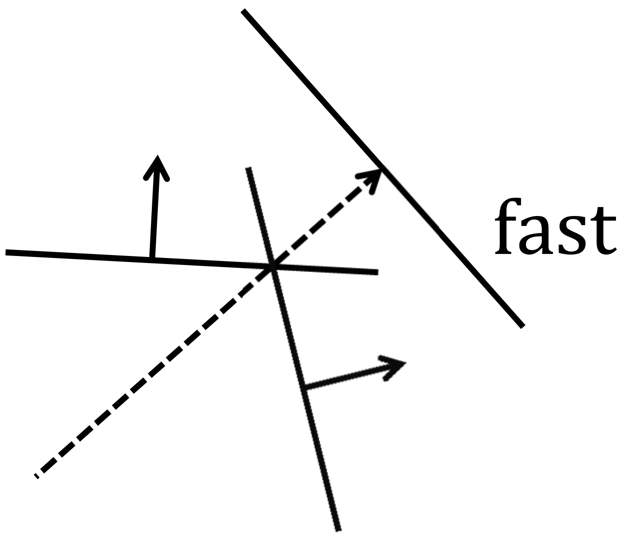
$$V = M(\vec{n})\sigma.$$

Large time asymptotics

Its asymptotic shape is W_M : Wulff shape of M, i.e.

$$W_m = \bigcap_{|m|=1} \{ x \mid x \cdot m \leq M(\vec{m}) \}$$

In other words, slow direction remains.



A surface with fast direction disappears.

Rigorous Statement

Thm (H. Ishii – G. Pires – P. E. Souganidis ’99)

Assume that M is continuous and $\sigma > 0$ is constant. If a compact set E_0 is bigger than the critical size, then its level-set flow $E(t)$ has the asymptotic

$$E(t) \,/\, t \to W_M \quad (t \to \infty)$$

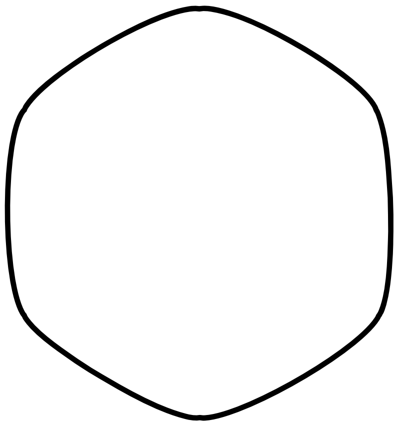
in the Hausdorff distance sense.

(n-dimensional result)

Physical explanation (continued)

For snow crystal W_M must be a regular hexagon in the plane. Thus snow flakes becomes a hexagon when it is very small.

A few problems (1) The asymptotic is a result by scaling down. So there may exist no real flat portion. Indeed, if the curvature effect exists, a corner is rounded and there is no flat portion by the strong maximum principle (if M is Lipschitz).



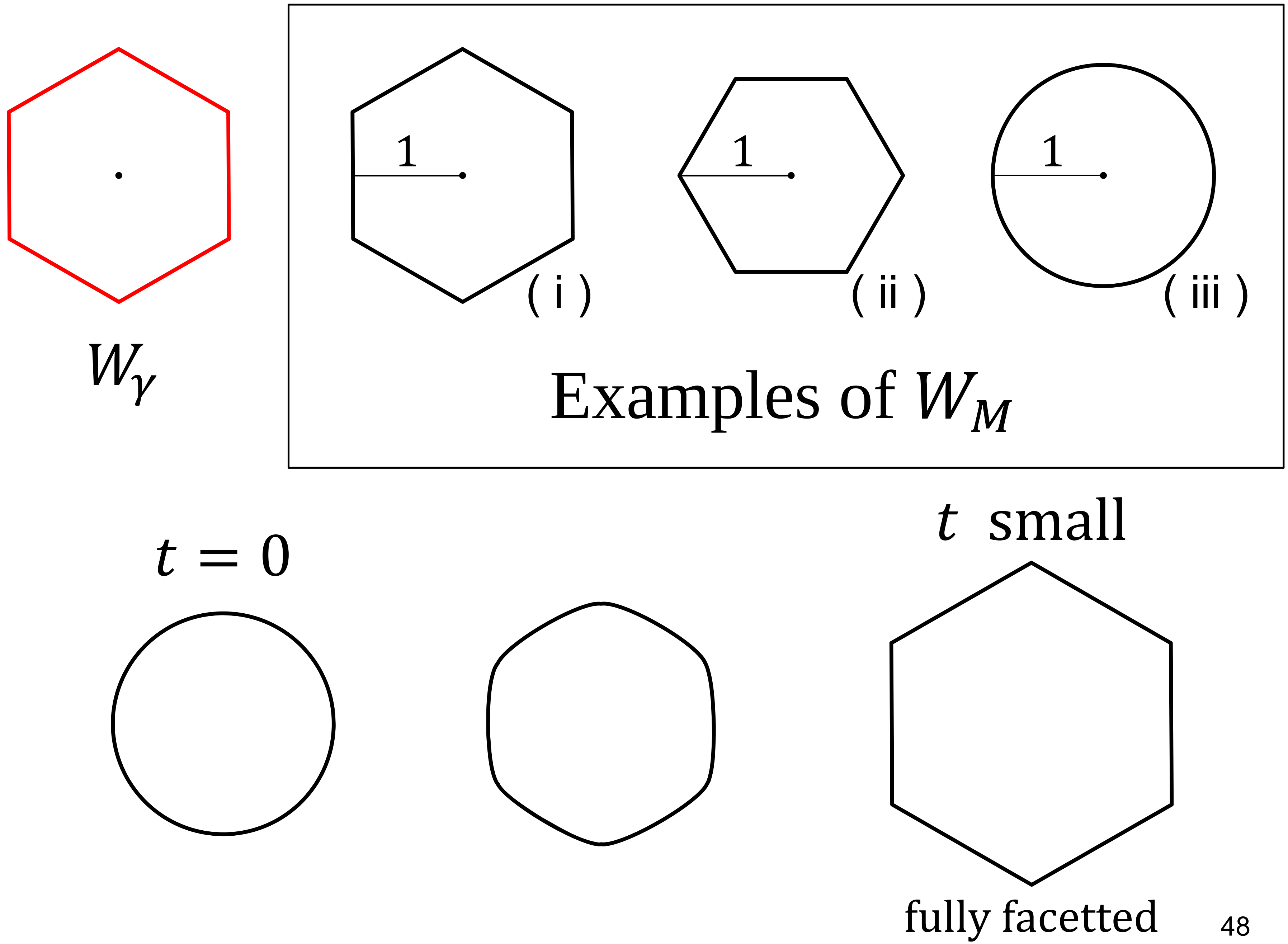
(2) In reality σ may not be constant.
(cf. recent computation by J. Barrett, H. Garcke and R. Nürnberg '11)

Does anisotropic curvature plays a little role?

Assume that the Wulff shape of γ is a regular polygon centered at zero. Assume that M is one in the direction of normals of W_γ. Assume that $\sigma > 0$ is a constant. Consider $V = M(\vec{n})\left(\kappa_\gamma + \sigma\right)$.

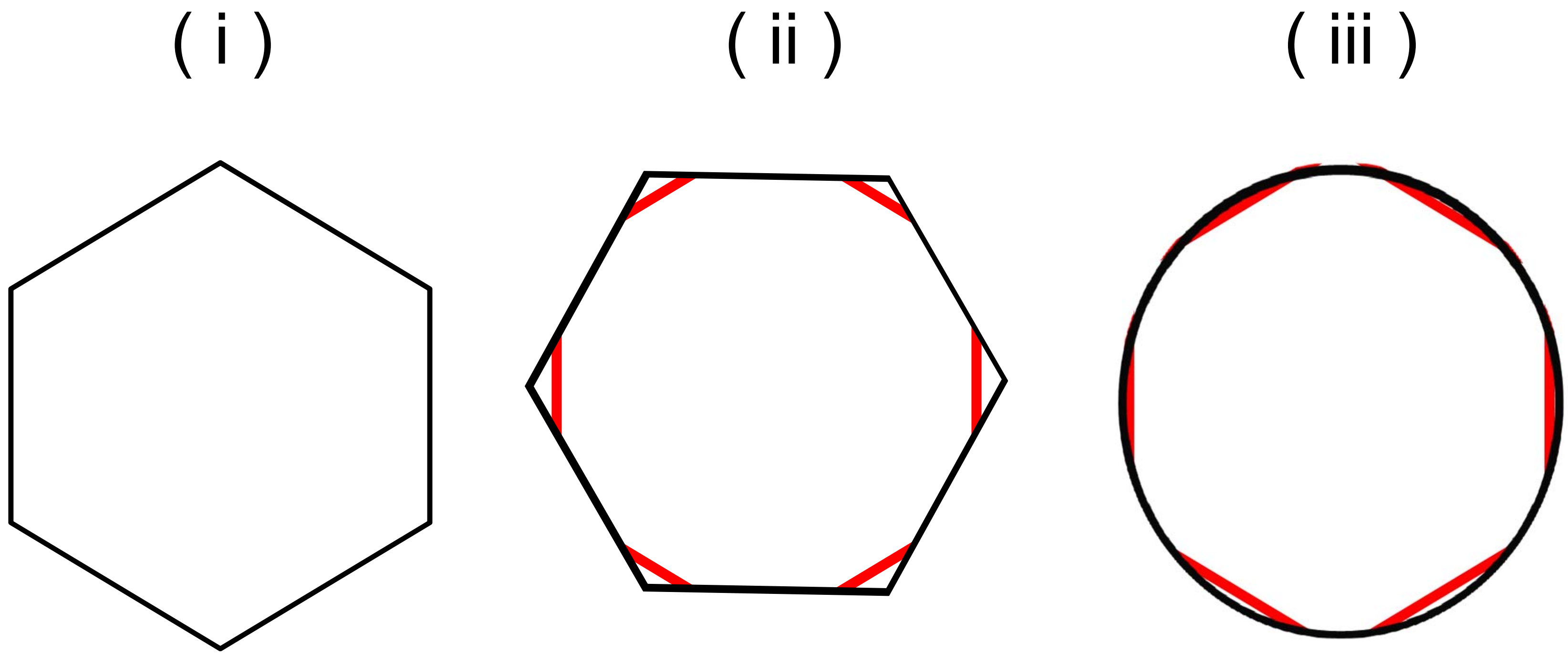
Thm (M.-H. Giga – Y. G., work in progress)

Assume that E_0 is a compact, convex set in $\mathbf{R}^2$. If initial data E_0 is bigger than a critical size and sufficiently close to the critical size, then its level set flow $E(t)$ becomes fully faceted with facets appeared in W_γ in finite time. If moreover E_0 and M have the 'same symmetry' as W_γ , then $E(t)$ becomes similar shape as W_γ .



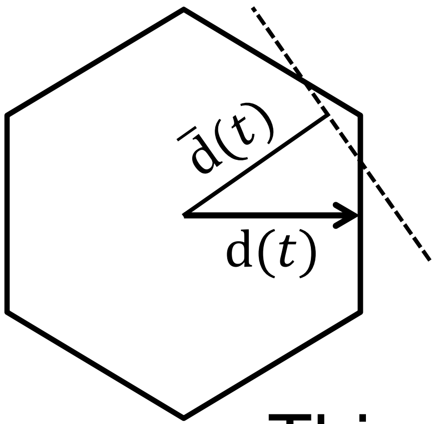
W_γ
1
(i)
1
(ii)
1
(iii)
Examples of W_M
$t = 0$
t small
fully facetted

t large



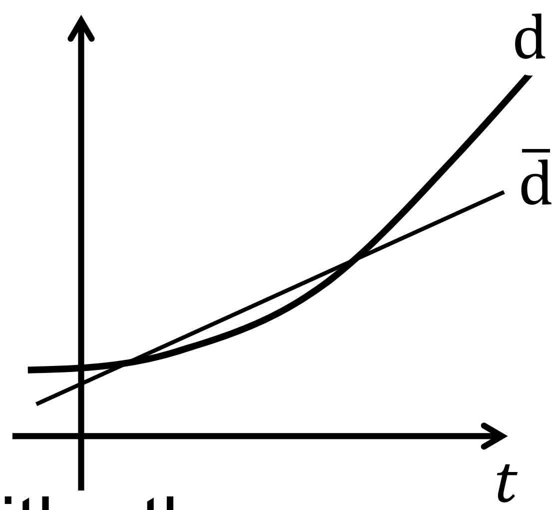
Ingredients of proofs

- Approximation by crystalline flow (use approximation theorem and consistency of level set and crystalline flows)
- Prove that a facet with normal different from Wulff moves very fast compared with other facets (everything is ODE)



Consider a self-similar solution of $V = \gamma(\kappa_\gamma + \sigma)$.

$$\dot{\mathrm{d}} = -\frac{\mathrm{const}}{\mathrm{d}} + \sigma$$



This gives an upper bound for facets with normals in Wulff (by comparison principle). A facet with other directions moves faster at least for a short time.

Remarks and further directions

- Even if σ depends on x, as far as $|\nabla\sigma|$ is small, then facet stays as a facet and speed : $V = -\mathrm{const}/\mathrm{length} + \sigma_{\mathrm{av}}$ where σ_{av} is the average of σ over the facet.

  (In fact, one is able to solve the Stefan type problem in 1.2; Y. G. – Rybka ’03. Also existence of a self-similar solution is known. Y. G. – Rybka ’05.)

- If $|\nabla\sigma|$ is not small, a facet may break, then the construction of solution itself is nontrivial. Explicit solutions are given for special cases (Y. G. – Rybka ’08, ’09, Y. G. – Rybka – Gorka ’10).

  A general viscosity theory is under construction.

Explanation

Crystal becomes fully faceted because of anisotropy of interfacial energy when it is small. Anisotropy of mobility plays a little role.

Consistent with Barrett – Garcke – Nürnberg’s simulation
(cf. R. Kobayashi – Y. G. ’01 JJIAM)

Summary

1. Several examples of very singular diffusion equations are discussed with their applications.
2. Characterization of evolution speed of a facet is given and it turns out that it is a nonlocal quantity.
3. A scale free extinction time estimate is given even for fourth order problems.
4. Well-posedness of initial value problem is disscussed.
5. For anisotropic curvature flow equations difference of role of two anisotropy (kinetic and interfacial) is explained.