INdAM Workshop “Nonconvex evolution problems”

Pattern formation & Partial Differential Equations

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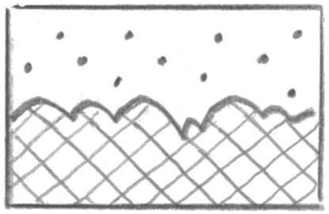
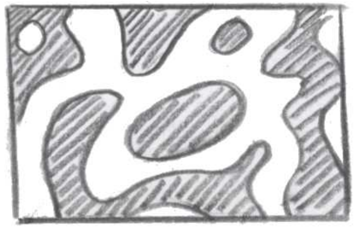
Pattern formation for two specific examples

A) crystal growth under deposition
— roughness of crystal surface



B) demixing of polymers
— labyrinth-like pattern
of concentration field



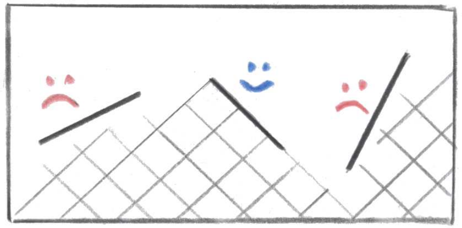
Few elementary mechanisms (diffusion, viscosity, ...)
— complex Pattern

Crystal growth and Kuramoto-Sivashinsky equation

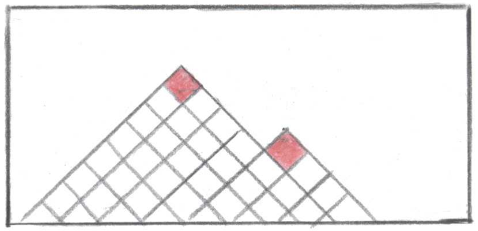
L. Giacomelli, D. Goldman

Relevant mechanisms

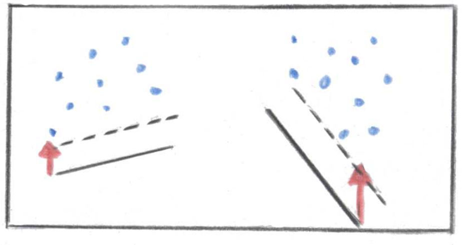
Crystal lattice favors certain slopes of the surface

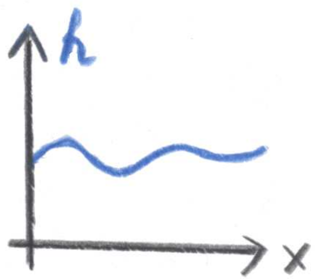


Exposed positions are disfavored



Vertical growth rate depends on slope





$$\frac{\partial h}{\partial t} = \underbrace{-\frac{\partial}{\partial x}((1-(\frac{\partial h}{\partial x})^2)\frac{\partial h}{\partial x})} \underbrace{-\frac{\partial^4 h}{\partial x^4}} \underbrace{+f\,(1+\frac{1}{2}(\frac{\partial h}{\partial x})^2)}$$

Qualitatively different behavior for small/large deposition rate f

Initial data $h(t = 0)$ $=$ white noise of small amplitude

Deposition rate $f \ll 1$

- slow growth
- facets with preferred slope ± 1
- number of facets decreases

Deposition rate $f \gg 1$

- fast growth
- slope $\ll 1$
- number of maxima/minima $\approx$ constant

“Convective” Cahn-Hilliard equation

Express equation for height h

$$\frac{\partial h}{\partial t} - f\,(1 + \tfrac{1}{2}(\frac{\partial h}{\partial x})^2) + \frac{\partial}{\partial x}((1 - (\frac{\partial h}{\partial x})^2)\frac{\partial h}{\partial x}) + \frac{\partial^4 h}{\partial x^4} = 0$$

in terms of slope $u = -\frac{\partial h}{\partial x}$

$$\frac{\partial u}{\partial t} + f\,\frac{\partial}{\partial x}(\tfrac{1}{2}u^2) + \frac{\partial^2}{\partial x^2}((1 - u^2)u) + \frac{\partial^4 u}{\partial x^4} = 0$$

For large deposition rate $f \gg 1$ rescale $u = \frac{1}{f}\hat{u}$:

$$\frac{\partial \hat{u}}{\partial t} + \frac{\partial}{\partial x}(\tfrac{1}{2}\hat{u}^2) + \frac{\partial^2}{\partial x^2}((1 - \frac{1}{f^2}\hat{u}^2)\hat{u}) + \frac{\partial^4 \hat{u}}{\partial x^4} = 0$$

Regime of strong deposition:
Kuramoto-Sivashinsky equation

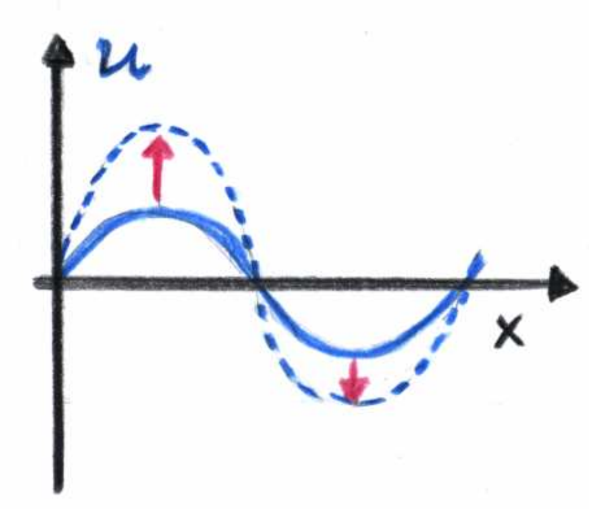
For $f \gg 1$, expressed in $u = -\frac{\partial h}{\partial x}$:

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\left(\frac{1}{2}u^2\right) + \frac{\partial^2 u}{\partial x^2} + \frac{\partial^4 u}{\partial x^4} = 0$$

Three terms — three simple mechanisms

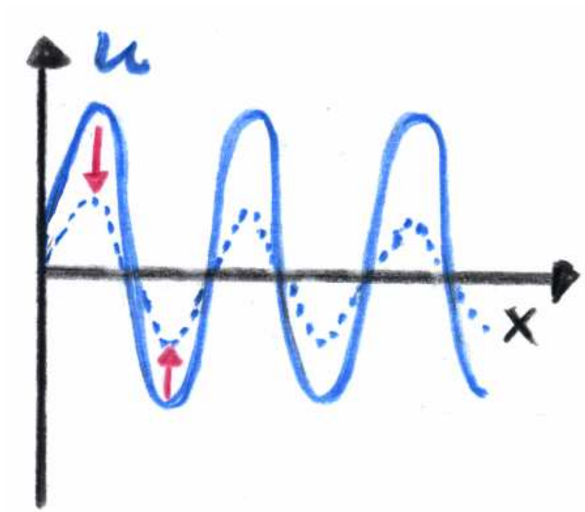
$$\frac{\partial^2 u}{\partial x^2}$$

Growth



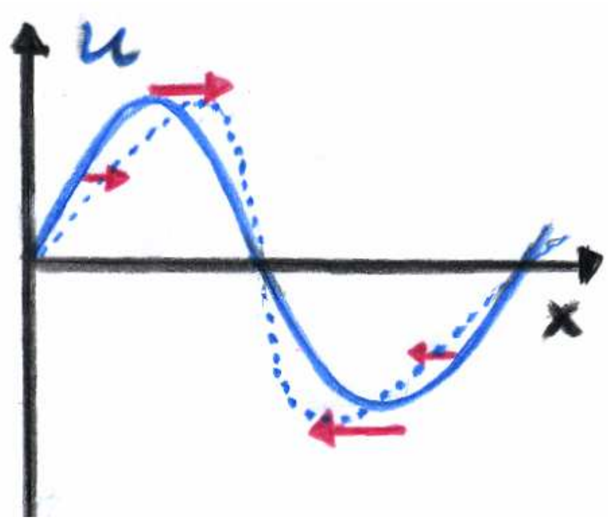
$$\frac{\partial^4 u}{\partial x^4}$$

Decay



$$\frac{\partial}{\partial x}\left(\tfrac{1}{2}u^2\right)$$

Shear



Periodic configurations $u(t, x + L) = u(t, x)$; large system $L \gg 1$

Dynamic equilibrium

Initial data: $u(t=0)$ = white noise of small amplitude

Observations:

Initial phase

- 1. Smoothing ($\frac{\partial^4 u}{\partial x^4}$)
- 2. Growth ($\frac{\partial^2 u}{\partial x^2}$)
- 3. Shear ($\frac{\partial}{\partial x}(\frac{1}{2}u^2)$)

Dynamic equilibrium

- average amplitude ~ 1
- average wave length ~ 1
- chaotic behavior in space & time

Shear contains exponential growth

Energy spectrum

Decomposition of spatial signal into waves of length $L, \frac{L}{2}, \frac{L}{3}, \cdots$:

$$(\mathcal{F}u(t,\cdot))(k) \;:=\; L^{-1}\int_0^L e^{ikx}u(t,x)\,dx \quad \text{(Fourier series)}$$

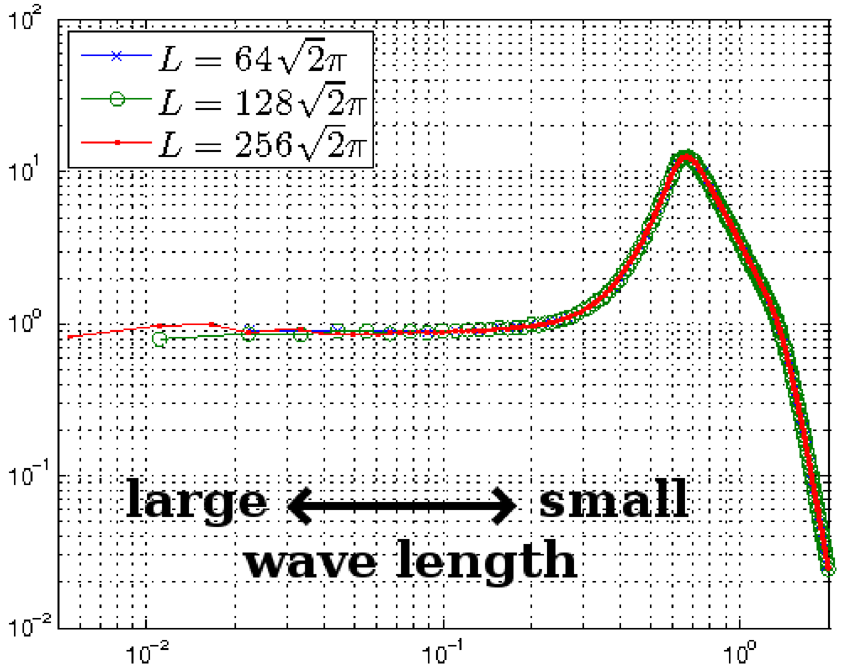
Contribution of wave number $(k, k+dk)$ to total energy:

$$L|(\mathcal{F}u(t,\cdot))(k)|^2\,dk$$

Time average:

$$\lim_{t_0\uparrow\infty} t_0^{-1}\int_0^{t_0} L|(\mathcal{F}u(t,\cdot))(k)|^2 dt$$

Equipartition of energy



Observations:

- Equipartition of energy over wave numbers $|k| \ll 1$
- Energy spectrum independent of $L \gg 1$

"Universal" behavior

Challenge for mathematics

Observation:
After initial phase, there is a dynamic equilibrium, with statistics independent of the initial data $u(t=0)$ and of the system size L

Challenge for theory of partial differential equations:
Why?

In mathematics: "Why ?" $=$ "**How can it be proved?**"

A good proof gives **insight** into "why"

Modest state of mathematical insight

Only statements of the following form have been proved:

space-time averages of $|u|$, $|\frac{\partial u}{\partial x}|$, $|\frac{\partial^2 u}{\partial x^2}| \lesssim \mathbf{1}$,

for all initial data $u(t=0)$, system sizes L

These statements have been proved step-by-step:

space-time averages of $|u|$, $|\frac{\partial u}{\partial x}|$, $|\frac{\partial^2 u}{\partial x^2}| \lesssim \mathbf{L^p}$,

for all initial data $u(t=0)$

Nicolaenko & Scheurer & Temam '85, Goodman '94: $\lesssim \mathbf{L^2}$

Collet & Eckmann & Epstein & Stubbe '93: $\lesssim \mathbf{L^{11/10}}$

Bronski & Gambill '06: $\lesssim \mathbf{L}$, Giacomelli & O. '05: $\ll \mathbf{L}$

O. '09 $\lesssim \ln^{\mathbf{5/3}} \mathbf{L}$

$\rightsquigarrow$ bounds on **dim**(Attractor), **dim**(Inertial Manifold), Fojas et. al.

Near-extensive bound

Theorem [O.,JFA '09]

For any $\sigma > 5/3$ there exists $C < \infty$ such that for all $L \geq 2$, all initial data $u(0)$ and $\alpha \in [\frac{1}{3}, 2]$ we have

$$\left(\lim_{T\uparrow\infty} T^{-1} L^{-1} \int_0^T \int_0^L \left| |\partial_x|^\alpha u \right|^2 dx\, dt \right)^{1/2} \leq C \ln^\sigma L.$$

Insight from proof

Three methods have been developed. Insight of last method:

Shear term $\frac{\partial}{\partial x}(\frac{1}{2}u^2)$ behaves like a *coercive* term, i. e.

$$\int_0^L \frac{\partial}{\partial x}(\frac{1}{2}u^2)\, u\, dx \quad \text{as} \quad \int_0^L \left| \left|\frac{\partial}{\partial x}\right|^{1/3} u \right|^3 dx$$

despite actually being *conservative*, i. e.

$$\int_0^L \frac{\partial}{\partial x}(\frac{1}{2}u^2)\, u\, dx \;=\; 0.$$

Conservative acts as coercive in forced inviscid Burgers

Consider $f(t,x)$, $g(t,x)$ with $\quad \frac{\partial u}{\partial t}+\frac{\partial}{\partial x}(\frac{1}{2}u^2) = \frac{\partial g}{\partial x}$, *smooth*, periodic in x, compactly supported in t. Then

$$\int\int\left|\left|\frac{\partial}{\partial x}\right|^{\frac{1}{3}}u\right|^3 dx\,dt \underset{\text{log}}{\overset{\lesssim}{\text{mod}}} \int\int\left|\left|\frac{\partial}{\partial x}\right|^{\frac{2}{3}}g\right|^{\frac{3}{2}} dx\,dt,$$

more precisely expressed in interpolation spaces

(Goldman & O.)

$$\|u;[\dot H^1_\infty, L_2]_{\frac{1}{3},\infty}\|^3 \lesssim \|g;[\dot H^1_2, L_1]_{\frac{2}{3},1}\|^{\frac{3}{2}}.$$

Connection with Onsager's conjecture on level of forced viscous Burgers

On the one hand, for $\frac{\partial u}{\partial t}+\frac{\partial}{\partial x}(\frac{1}{2}u^2)-\nu\frac{\partial^2 u}{\partial x^2}=\frac{\partial g}{\partial x}$ have *uniform estimate* in $\nu\downarrow 0$

$$\|u;[\dot H^1_\infty,L_2]_{\frac{1}{3},\infty}\|^3+\nu\|u;\dot H^1_2\|^2\lesssim\|g;[\dot H^1_2,L_1]_{\frac{2}{3},1}\|^{\frac{3}{2}}.$$

On the other hand, at $\nu=0$ if $u\in[\dot H^1_\infty,L_2]_{\frac{1}{3},p}$ with $p<\infty$, would have *conservation of energy*

$$\frac{d}{dt}\int\frac{1}{2}u^2\,dx=\int u\frac{\partial g}{\partial x}\,dx.$$

B. Demixing and Cahn-Hilliard equation

R. V. Kohn, Brenier & Seis, Seis & Slepcev

Cahn–Hilliard equation

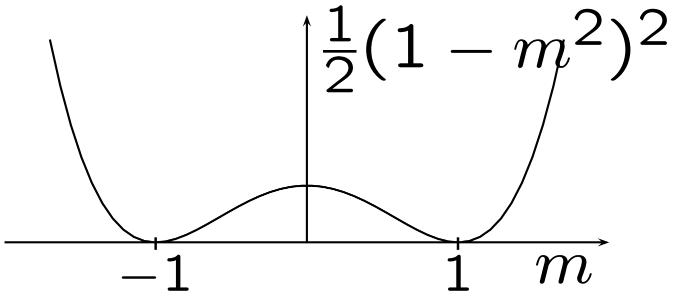
conserved order parameter:

$\partial_t m + \nabla \cdot j \; = \; 0$

diffusion flux: $\; j \; = \; -\nabla \frac{\partial E}{\partial m}$

free energy: $E(m)$

$= \; \int \frac{1}{2}|\nabla m|^2 + \frac{1}{2}(1 - m^2)^2 \, dx$



periodic b.c. in $(0, L)^n$ with $L \gg 1$

Cahn–Hilliard equation with flow

Fluid flow next to diffusion

$$\partial_t m + \nabla \cdot j + \nabla \cdot (mu) \;=\; 0$$

where $j = -\lambda \nabla \frac{\partial E}{\partial m}$ and velocity u is determined by Stokes

$$-\triangle u + \nabla p \;=\; -m \nabla \frac{\partial E}{\partial m} \quad \text{and} \quad \nabla \cdot u \;=\; 0$$

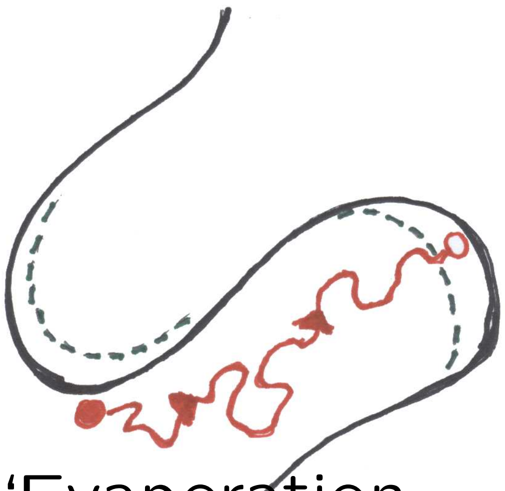
Non-dimensional mobility parameter $\lambda \gg 1$

Thermodyn. consistent: $\frac{dE}{dt} = -\frac{1}{\lambda} \int |j|^2 \, dx - \int |\nabla u|^2 \, dx$

Dissipation mechanism influences dynamics

Energy functional $E \approx \frac{4}{3}$area of transition layer

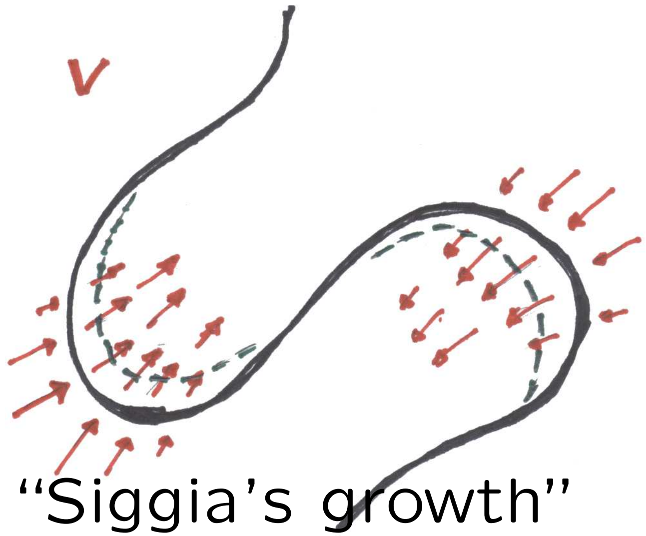
mediated by diffusion,
limited by outer friction



“Evaporation-

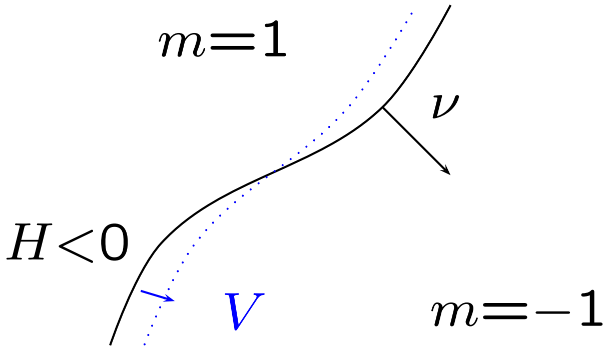
Recondensation”

mediated by flow,
limited by viscosity



“Siggia’s growth”

Geometric evolution equation, diffusion only



mean curvature: H

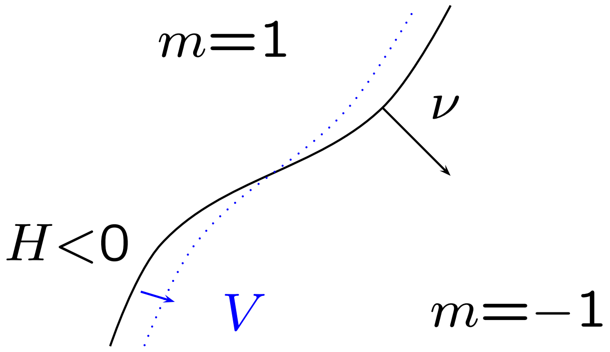
normal velocity: V

$$-\triangle\mu = 0 \quad \text{in bulk,} \quad \left\{ \begin{array}{lcl} \mu & = & \frac{2}{3}H \\ V & = & [\nu\cdot\nabla\mu] \end{array} \right\} \text{ on interface}$$

"Mullins-Sekerka" ; Pego, Alikakos&Bates&Chen, Röger & Schätzle

Third-order free boundary problem

Geometric evolution equation, flow only



$$\left\{\begin{array}{rcl} \nabla\cdot u &=& 0 \\ -\nabla\cdot S &=& 0 \end{array}\right\} \text{ in bulk,} \qquad \left\{\begin{array}{rcl} \tau\cdot[S]\nu &=& 0 \\ \nu\cdot[S]\nu &=& -\frac{4}{3}H \\ V &=& \nu\cdot u \end{array}\right\} \text{ on interface,}$$

where $S := \frac{1}{2}(\nabla u + \nabla^t u) - p\,\mathrm{id}$ is stress tensor

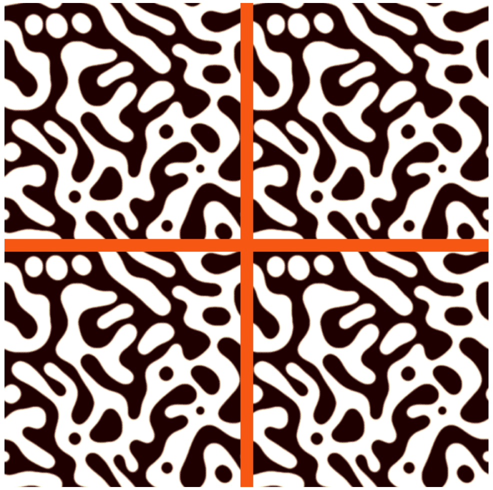
First-order free boundary problem

Statistical self-similarity

earlier

later

later,
rescaled,
periodically
extended



Diffusion dominated: coarsening exponent 1/3

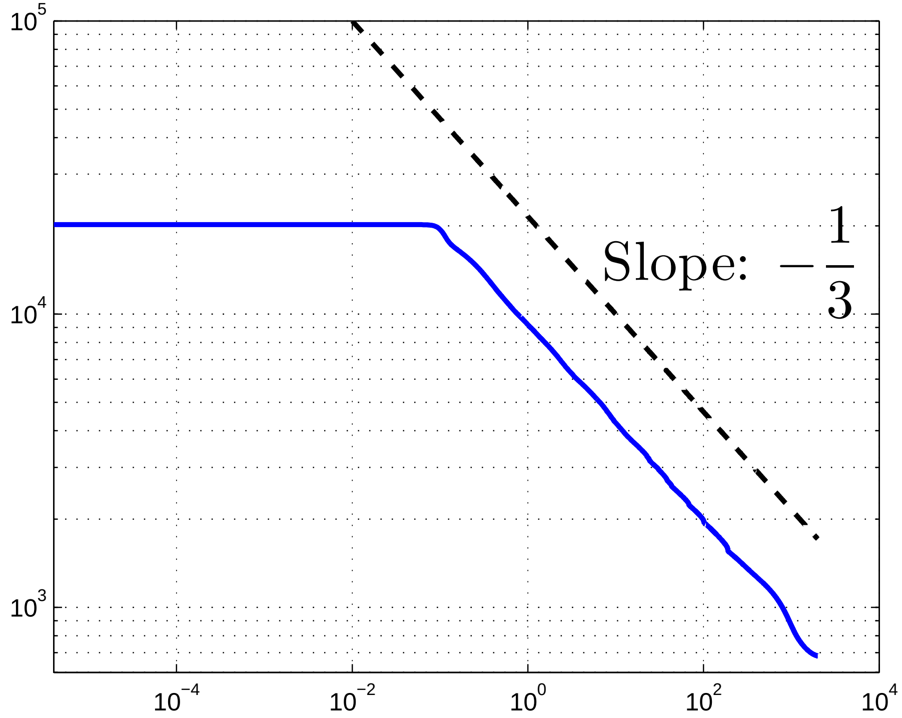
After initial phase: Energy $E(m) \approx \frac{4}{3}$area of transition layer

Hence $\left(\frac{1}{L^n}E(m)\right)^{-1}$ is an *average length scale*

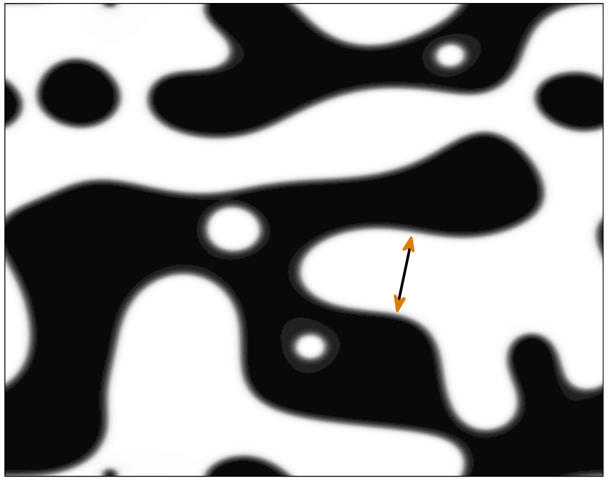
Energy E vs. time t,

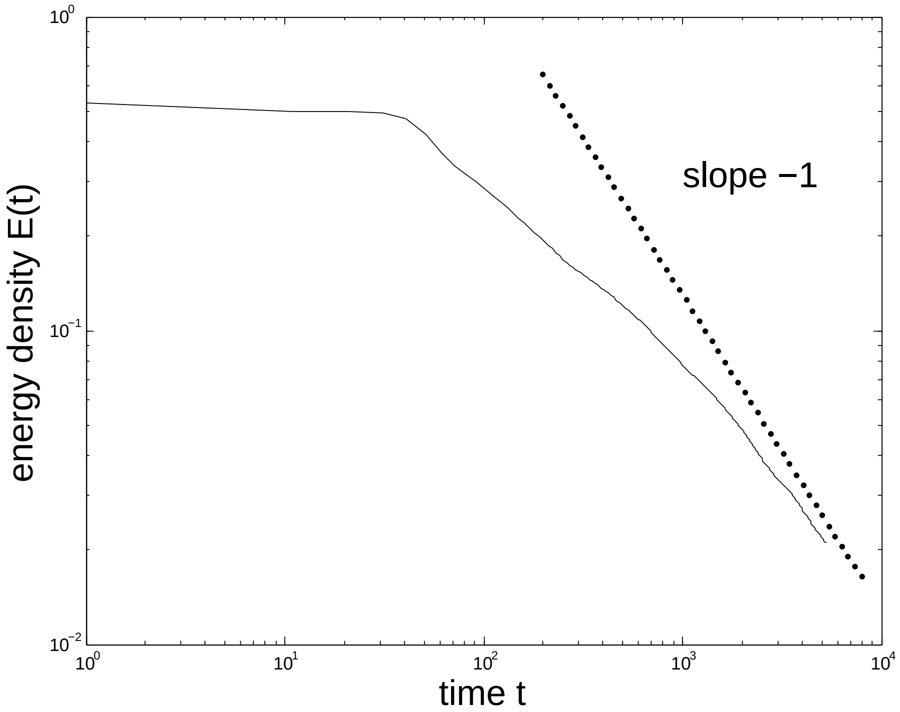
double logarithmic plot:

$$\mathbf{L^{-(n=2)}E(m) \sim t^{-1/3}}$$



Flow dominated: coarsening exponent 1

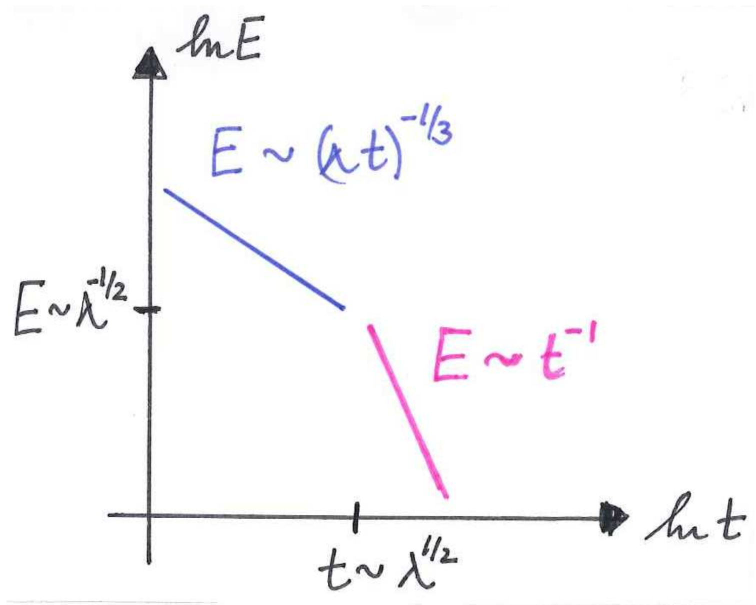




$$\mathbf{L^{-(n=2)}E(u) \sim t^{-1}}$$

Cross-over from $t^{-1/3}$ to t^{-1}

Heuristics(Siggia '79): *Faster* mechanism dominates



initially: Diffusion faster

later: Flow faster

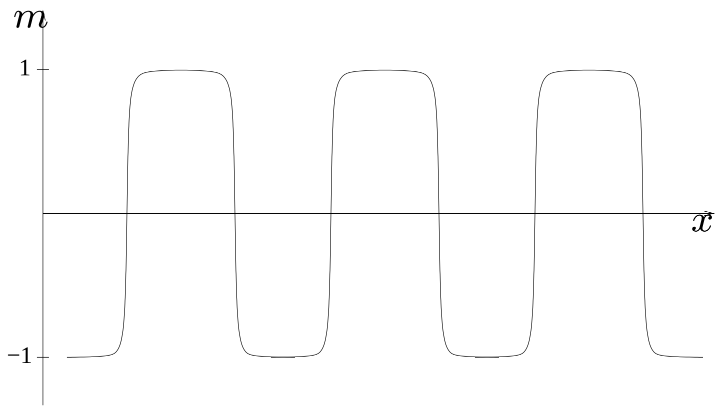
... confirmed by experiments

Rigorous treatment

has to cope with ungeneric behavior

Upper bounds on E not independent of initial data:

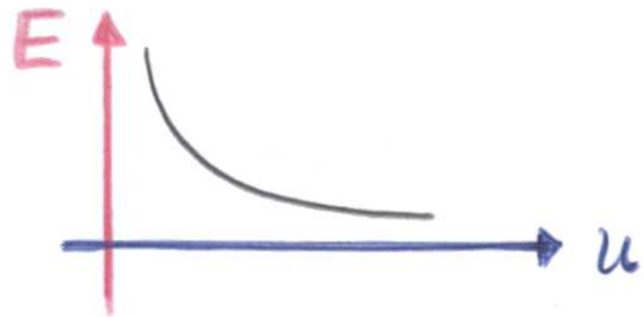
— too many stationary points of E



Lower bounds on E independenty of initial data

Basic idea for rigorous lower bounds on E

Dynamics is steepest descent
in energy landscape

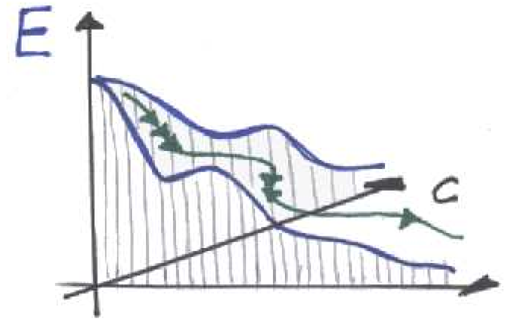


energy	$\leftrightarrow$	heights,
dissipation mechanism	$\leftrightarrow$	distances

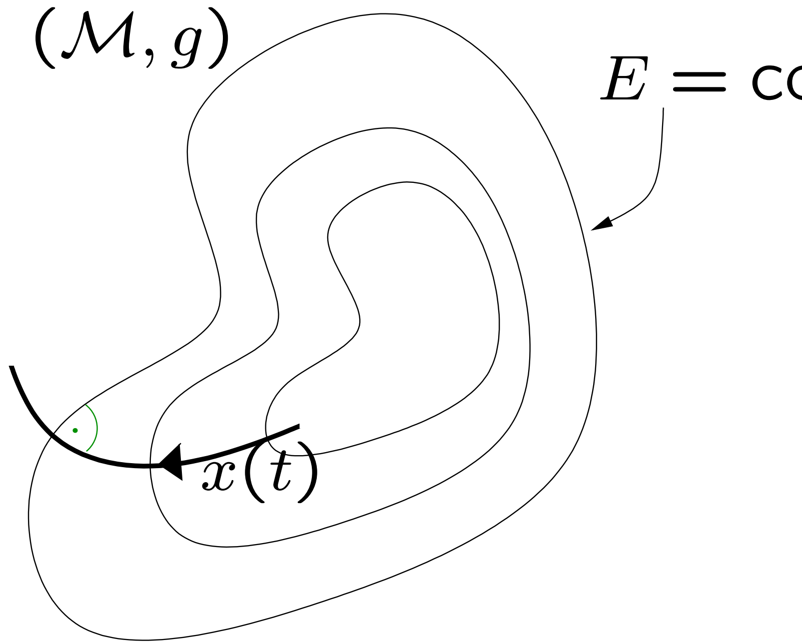
landscape *not steep*

$\Longrightarrow$

energy decreases *not fast*



An abstract framework



$(\mathcal{M}, g)$	Riemannian manifold
E	functional on $\mathcal{M}$

Gradient flow $\dot{x} = -\mathrm{grad}_g E(x)$

metric tensor $g_x(\delta x, \delta x)$ $\rightsquigarrow$ induced distance $d(x_0, x_1)$

local *global*

Relating geometry to dynamics

Lemma. (Kohn & O. '02)

Assume for some $\alpha > 0$ and $x^* \in \mathcal{M}$

$$E(x) \gtrsim d(x^*, x)^{-\alpha} \quad \text{provided } E(x) \leq 1$$

Then for all $\sigma \in (1, \frac{\alpha+2}{\alpha})$

$$\int_0^T E(x(t))^\sigma \, dt \gtrsim \int_0^T (t^{-\frac{\alpha}{\alpha+2}})^\sigma \, dt \qquad \text{for } T \gg d(x^*, x(0))^{\alpha+2} \text{ and } E(x(0)) \leq 1.$$

Type of dissipation determines metric tensor g

Transport mechanism		type of dissipation:
diffusion	$\rightsquigarrow$	outer friction,
flow	$\rightsquigarrow$	inner friction (viscosity).

$$
\begin{aligned}
& g_m(\delta m, \delta m) \\
& \quad = \ \inf \Big\{ \frac{1}{\lambda} \int |j|^2 \, dx + \int |\nabla u|^2 \, dx \ \Big| \\
& \qquad \qquad \delta m + \nabla \cdot j + \nabla \cdot (m\, u) \ = \ 0, \ \nabla \cdot u \ = \ 0 \Big\}.
\end{aligned}
$$

... but induced distance d not explicitly known

Lower bound D

on induced distance d to reference configuration m^*

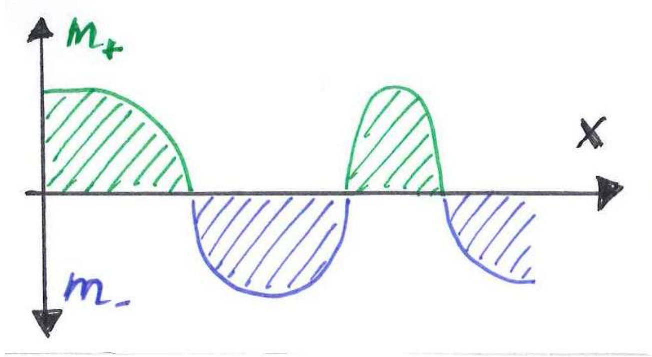
Reference configuration: well-mixed state $m^* = 0$

Lower bound $D(m)$ to **induced distance** $d(m, m^*)$

given by **transportation distance**

between $m_+ := \max\{m, 0\}$

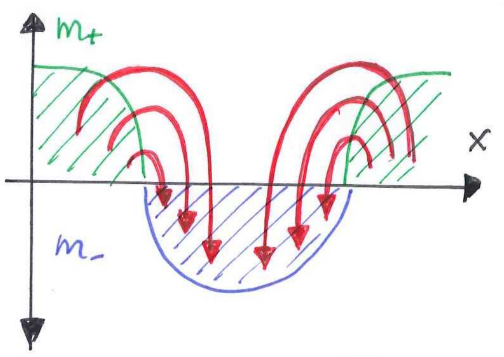
and $m_- := \max\{-m, 0\}$

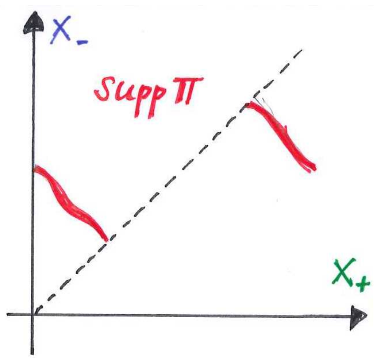


Definition of transportation distance D

Given $m = m_+ - m_-$, measure $\pi(dx_- \, dx_+)$ on $[0,L]^n \times [0,L]^n$ is called **admissible transfer plan** provided

$$\begin{aligned} \int \zeta(x_+)\,\pi(dx_+\,dx_-) &= \int \zeta(x)\,m_+(x)\,dx, \\ \int \zeta(x_-)\,\pi(dx_+\,dx_-) &= \int \zeta(x)\,m_-(x)\,dx. \end{aligned}$$

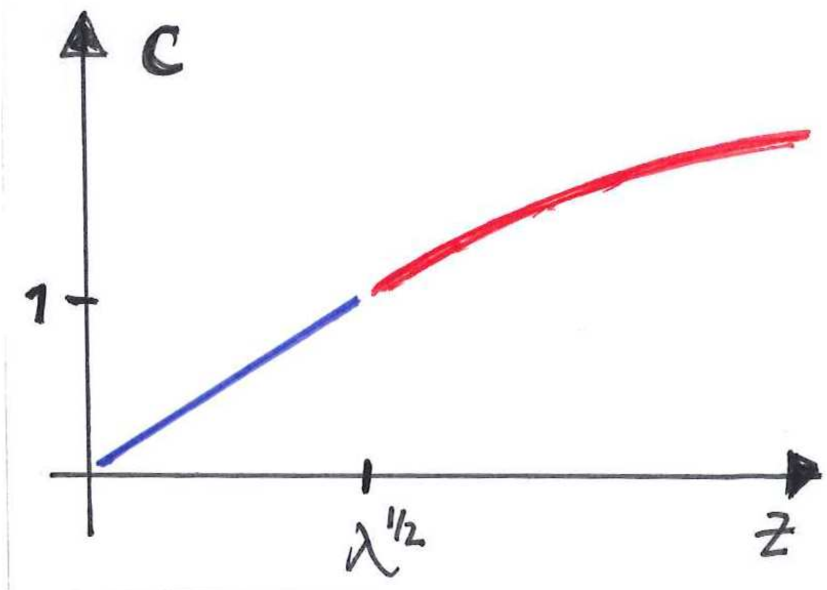




$$\mathbf{D}(\mathbf{m}) \; := \; \inf\left\{ \int \mathbf{c}(|x_- - x_+|)\pi(dx_+\,dx_-) \;\middle|\; \pi \text{ admissible} \right\}$$

Choice of cost c

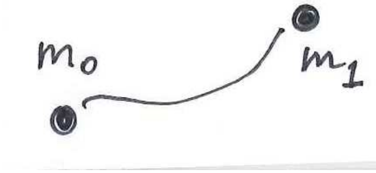
cross-over between **linear** and **logarithmic** at $z = \lambda^{1/2}$

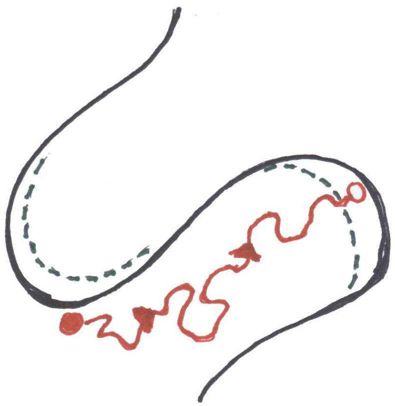


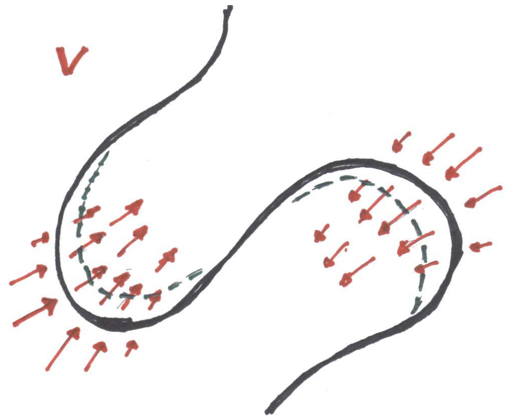
$$\mathbf{c(z)} := \begin{cases} \frac{z}{\lambda^{1/2}} & \text{for } z \leq \lambda^{1/2} \\ 1 + \ln \frac{z}{\lambda^{1/2}} & \text{for } z \geq \lambda^{1/2} \end{cases}$$

Dissipation mechanism determines geometry

Distance on configuration space







diffusion

transportation distance with cost

$c(x_- - x_+)$

$= |x_- - x_+|$

flow

transportation distance with cost

$c(x_- - x_+)$

$= \ln(1 + |x_- - x_+|)$

Main result

Theorem. (O. & Seis & Slepcev '10+, Brenier, O. & Seis '10)

For any solution u with $\lambda \gg 1$, $L \gg 1$,

$$\int_0^T \max\{\lambda^{\frac{1}{2}}(\frac{E}{L^n})^2, \frac{E}{L^n}\}\, dt \ \gtrsim \ \min\left\{\left(\frac{T}{\lambda^{\frac{1}{2}}}\right)^{1/3}, 1 + \ln(1 + \frac{T}{\lambda^{\frac{1}{2}}})\right\}$$

provided

$$\frac{E(0)}{L^n} \lesssim 1 \quad \text{and} \quad \frac{T}{\lambda^{\frac{1}{2}}} \gg \left(\frac{D(0)}{\lambda^{\frac{1}{2}}}\right)^3 \ (\gtrsim 1).$$

Dissipation: $D(m)$ is lower bound to $d(m, m^*)$

Dissipation Lemma (BOS, OSS).

Suppose

$$\partial_t m + \nabla \cdot j + \nabla \cdot (mu) = 0,$$
$$\nabla \cdot u = 0.$$

Then provided $\frac{1}{L^n} E(m) \lesssim 1$

$$\left(\frac{1}{L^n} \frac{d}{dt} D(m) \right)^2 \lesssim \lambda^{-1} \frac{1}{L^n} \int |j|^2 dx + \frac{1}{L^n} \int |\nabla u|^2 dx.$$

Uses idea of Crippa-DeLellis ('08)

for quantification of DiPerna-Lions theory

on uniqueness for transport equations $\partial_t m + u \cdot \nabla m = 0$

Future directions

Local estimates

Example with cross-over due to dissipation mechanisms

"in series", like diffusion+attachment-limited

— instead of "in parallel", like diffusion+flow-mediated (Dai&Pego on LSW-level)

Future directions

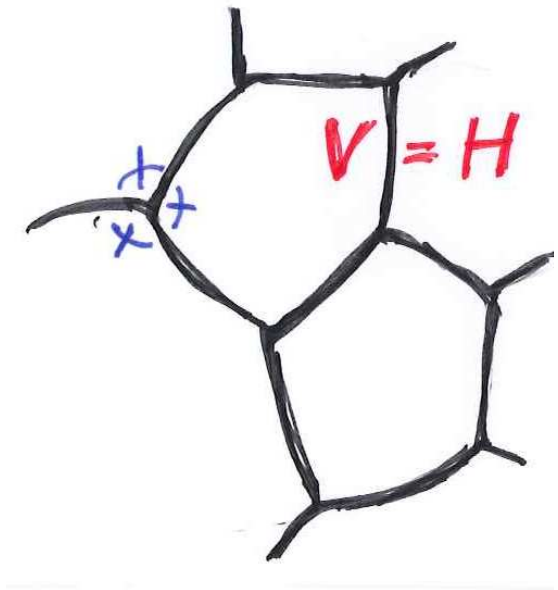
Grain growth

= aging in polycrystals

= multi-component

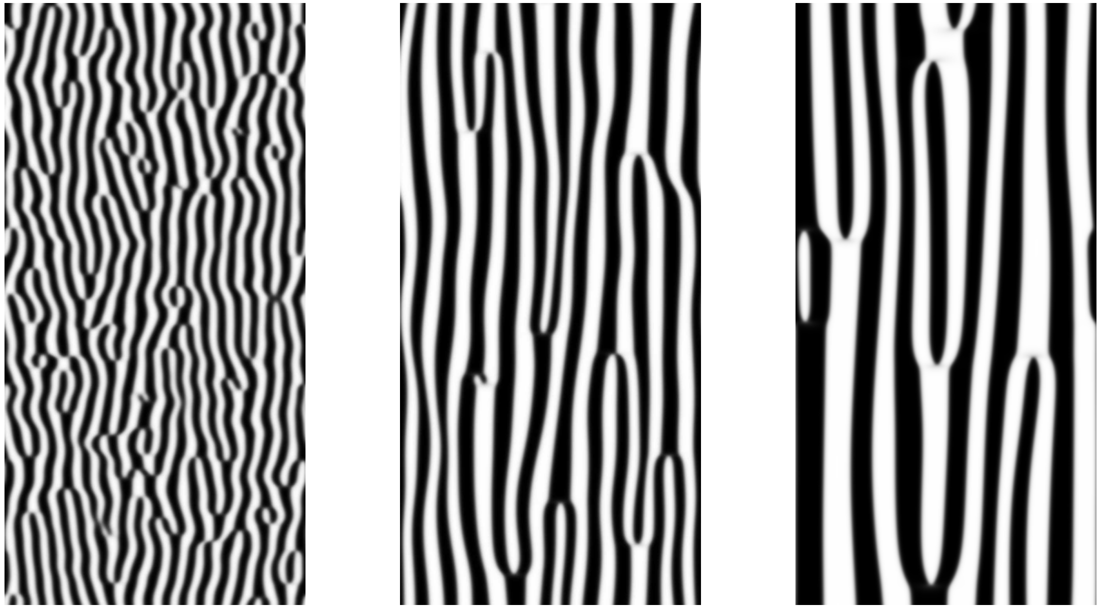
mean curvature flow

$\frac{1}{L^n} E \gtrsim t^{-1/2}$



Future directions

Defect-mediated coarsening (e.g. in Siegert's model for crystal growth)



Upper bounds on E for *generic* initial data