R. Kohn – Lecture 1 (CMU): Bounds on Coarsening Rates

Outline:

(1) Focus on "motion by surface diffusion". Energy-driven. Natural conjecture: length scale $\sim t^{1/4}$. Why is this hard?

(2) Kohn-Otto scheme for 1-sided bound on coarsening rate: uses E = energy, L = length scale, measured via neg Sobolev norm. Main ingredients: (a) "interpolation inequality", (b) "energy inequality", (c) "ODE lemma"

(3) if time permits: discuss briefly some other applns of this method

Related reading:

- method 1st introduced in Kohn + Otto, Comm Math Phys 229 (2002) 375-395 (this paper focuses on diffuse rather than sharp interface models)

- other early applns include multicomponent phase separation + an epitaxial growth model, see Kohn + Yan CPAM 56 (2003) 1549-1564 + Interf. + Free Bound. 6 (2004) 135-149

- Recent paper by Otto, Rump, + Slepcev, SIAM J. Math Anal 38 (2006) 503-529 considers rather different appl'n (liquid droplets on 2D surface) + also explains existence of a natural choice for "length scale" $L(t)$

- Other recent appl'ns: mean field theories of Ostwald ripening (Dai + Pego, SIAM J Math Anal. 37, 2005, 347-371; also nicely presented in Pego's lecture notes CMU-CNA preprint 06-CNA-001); Mullins-Sekerka in low vol fr limit (Conti, Niethammer, Otto, SIAM J Math Anal 38, 2006, 503-529); discrete evolutions modeling aggregation (in population dynamics) & denoising (in computer vision), Greer + Esedoglu, preprint avail at Esedoglu's website.

Focus, to be specific, on "motion by surface diffusion" in 2D

$\Gamma(t)$ = evolving curve in plane
normal velocity = $\partial_{ss} K$ $\quad$ K = curvature

$t = 1$ $\quad$ $t = 2$ $\quad$ $t = 10$

Pix show spatially periodic simulation with "random" initial data (from Puri, Bray, Lebowitz, Phys Rev E, 1997)

Common belief:

- length scale coarsens, $l(t) \sim t^{1/4}$
- soln is "statistically self-similar" (after initial transient, + before finite-size effects become important).

Note: evolution is "energy-driven" in the sense that it is a gradient system, namely "steepest descent for perimeter, wrto H_Γ^{-1} inner product." Explain: if κ = curvature + V = nor velocity then

$$\frac{d}{dt}\text{Perimeter} = \int_\Gamma \kappa V_{nor} = \langle \partial_s \kappa, \partial_s V_{nor} \rangle_{H^{-1}(\Gamma)}$$

for any evolution of Γ. So $-\partial_{ss}\kappa$ is the "gradient" of perimeter wrto $H^{-1}(\Gamma)$ inner product.

If preceding calcn is confusing, don't worry: we won't use it explicitly. But note more elementary facts:

- Perimeter decreases since $\frac{d}{dt}\text{Perimeter} = -\int_\Gamma |\partial_s \kappa|^2 ds$

- vol of each phase is preserved since
$$\frac{d}{dt}\,\mathrm{vol} = \int_\Gamma v_{nor}\,ds = \int_\Gamma \kappa_{ss}\,ds = 0.$$

You might worry abt whether flow is globally well-defined. Proper fix is to use diffuse-interface model ("Cahn-Hilliard with degenerate mobility"). Stick to sharp-interface version here, for simplicity.

Why should coarsening rate be $t^{1/4}$? Well, motion law is invt under $x \to \lambda x$, $t \to \lambda^4 t$. So if there's <u>any</u> power law it must be 1/4.

<u>Why is this difficult</u>?

- conjectured self-similarity might be false; at least, it depends on meaning of "random initial data"

  → Don't attempt that. Focus just on the "coarsening rate"

- assertion that $l(t) \sim t^{1/4}$ really says two things

a) "configuration must coarsen <u>at least</u> this fast"

b) "configuration doesn't coarsen faster"

(a) is <u>false</u> in general (eg spherical regions of black in matrix of white)

$\Rightarrow$ if true for solns, requires info on initial data + how geometry evolves.
NO PROGRESS HERE

(b) is different: true universally. So accessible by pde methods.
THIS IS MAIN FOCUS OF LECTURE.

<u>Recall goal, discuss plan of attack:</u>

We'd like to show $\ell(t) \le C t^{1/4}$, where

$\ell(t)$ = suitably defined "length scale of pattern"

Actually, we achieve less: just a time-averaged version of desired bd (details later).

<u>Basic ingredients</u>

① How to measure "length scale of pattern"? Two alternatives: one is

$$E(t) = \frac{\text{Perimeter in period cell}}{\text{Vol of period cell}} = ⨍|\nabla \chi|$$

(scales like 1/length). The other is to use a neg sobolev norm, such as

$$L(t) = \max_{\substack{|\nabla g| \le 1 \\ \text{periodic}}} ⨍ g(\chi - \bar{\chi})$$

(dual to $W^{1,\infty}$, so we sometimes express this formally as $L = ⨍|\nabla^{-1}(\chi - \bar{\chi})|$).

Here $\chi = \begin{cases} +1 & \text{in one phase} \\ -1 & \text{in other phase} \end{cases}$

② E + L are related by an "interpolation inequality"

$$E \cdot L \ge \text{constant}$$

(this is "just calculus" ie it has nothing to do with eqn of motion)

③ time rates of change are related

$$\left(\frac{dL}{dt}\right)^2 \leq CE \left| \frac{dE}{dt} \right|$$

(this is an "energy inequality", reflecting the dissipative dynamics)

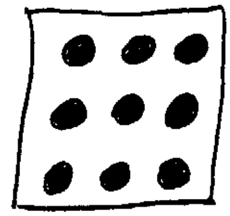
④ Extract desired bd (or closest we can come to it) from ② + ③ by elementary ODE argument.

Discuss these ingredients, each in turn. Start with $E(t)$ vs $L(t)$.

(Spatial averaging is crucial here. We assume periodicity to make it easy. But we'll be careful that size of period cell should not enter into est of coarsening rate.)

Gain intuition abt E+L by considering simple periodic geometry:

N inclusions, local length scale ℓ, vol fr $1/2$



then $E = \frac{\text{Perim}}{\text{cell area}} \sim \frac{N\ell}{N\ell^2} \sim \frac{1}{\ell}$;

as for $L = \max_{|\nabla g| \le 1} \int \chi g$, it prefers

g = largest ($g \sim \ell$) in centers ($\chi = 1$)
g = smallest ($g \sim -\ell$) in matrix ($\chi = -1$).

$\Rightarrow$ typical value of $\int \chi g$ is about ℓ.

Use of E was obvious: evolution is "energy driven" (E is a Liapunov fnl)

Use of L is less obvious; in fact, for many applns a different neg norm would do just as well, for example "H^{-1} norm," defined by

alternate
$$L(t) = \sup_{\int |\nabla g|^2 \le 1} \int (\chi - \bar{\chi}) g$$
$$= \left(\int |\nabla \Delta^{-1} (\chi - \bar{\chi})|^2 \right)^{1/2}$$
$$= \| \chi - \bar{\chi} \|_{H^{-1}}$$

Next, discuss "interpolation inequality"

$$(*) \qquad E \cdot L \geq \text{constant}$$

This is a consequence of the more general relation

$$(**) \qquad \int |u| \leq C \left(\int |\nabla u| \right)^{1/2} \left(\int |\nabla^{-1} u| \right)^{1/2}$$

for any periodic u with mean value 0.
Applying it to $u = \chi - \bar{\chi}$, we see that the constant on RHS of $(*)$ $\to 0$ as vol fr of either phase $\to 0$ (opt'l dependence of const in $(*)$ upon vol fr is discussed in recent paper by Choksi, Conti, Kohn, Otto, CPAM 2008).

Pf of $(**)$ is quite elementary. Here's a sketch:

Let u_δ = convolution of u with standard mollifier at scale δ. Then

$$\int |u - u_\delta| \leq \sup_{|h| \leq \delta} \int |u(x) - u(x+h)|$$
$$\leq C\delta \int |\nabla u|$$

also

$$\int |u_\delta| = \sup_{|g| \leq 1} \int u_\delta g$$
$$= \sup_{|g| \leq 1} \int u g_\delta$$
$$\leq \frac{C}{\delta} \int |\nabla^{-1} u| \qquad \text{since } \|\nabla g_\delta\|_{L^\infty} \leq \frac{C}{\delta} \|g\|_{L^\infty}$$

So $$\int |u| \leq C\left[\delta \int |\nabla u| + \frac{1}{\delta} \int |\nabla^{-1} u|\right]$$

Optzn over δ now gives (**).

Next, the "energy inequality". Like all energy inequalities, it's elementary.

Fix g st $|\nabla g| \leq 1$. Then

$$\frac{d}{dt} \int (\chi - \bar{\chi}) g = \frac{2}{|Q|} \int_\Gamma V_{nor}\, g \qquad Q = \text{unit cell}$$

$$= \frac{2}{|Q|} \int_\Gamma \partial_{ss} K \cdot g$$

$$= -\frac{2}{|Q|} \int_\Gamma \partial_s K \, \partial_s g$$

$$\le 2 \left(\frac{1}{|Q|} \int_\Gamma (\partial_s K)^2 \right)^{1/2} \left(\frac{1}{|Q|} \int_\Gamma 1 \right)^{1/2}$$

Since $\frac{d}{dt} E = -\frac{1}{|Q|} \int_\Gamma |\partial_s K|^2$, this gives

$$\frac{d}{dt} \int (\chi - \bar{\chi}) g \le C E^{1/2} \left(\frac{dE}{dt} \right)^{1/2}$$

Letting g be optimal (now g depends on t, but terms on LHS assoc g_t vanish by optimality) we get

$$\frac{dL}{dt} \le C E^{1/2} \left(\frac{dE}{dt} \right)^{1/2}$$

as asserted. (Hypoth that opt'l g is diff'ble in t can be avoided; see eg Kohn-Otto CMP paper.)

Finally, extraction of desired bds by

ODE argument.

Basic idea is clear: if our inequalities were actually equalities, say

$$EL = 1 \quad \text{and} \quad \dot{L} = E^{1/2}|\dot{E}|^{1/2}$$

then elementary manipulation would give $\dot{L} = L^{-3}$, whence $\frac{1}{4}(L^4(t) - L^4(0)) = t$. So $L \sim t^{1/4}$ at large times.

One could hope that when both relns are inequalities

$$EL \geq 1 \quad , \quad \dot{L} \leq E^{1/2}|\dot{E}|^{1/2}$$

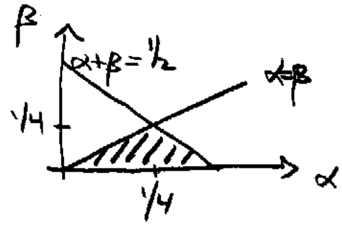
(ignoring constants) preceding we could still get a 1-sided result

$$(***) \qquad E \geq Ct^{-1/4} \quad , \quad L \leq Ct^{1/4} \quad \text{for large } t.$$

Alas, (***) does not follow from the available inequalities. For example: $L \geq Ct^{1/4}$ cannot follow, because if $L(t) = t^{\alpha}$ and $E(t) = t^{-\beta}$ then

$$EL \geq 1 \implies 0 \leq \beta \leq \alpha$$

$$\dot{L} \le |\dot{E}|^{1/2} E^{1/2} \Rightarrow \alpha+\beta \le 1/2.$$



Thus: no concl should be possible for $L(t)$.
But perhaps we can still show $E \ge Ct^{-1/4}$?

Actually, ptwise est of that type is also false! But a time-averaged est is true: our inequalities imply

(****) $$\frac{1}{T}\int_0^T E^3(t)\,dt \ge C \cdot \frac{1}{T}\int_0^T \left(t^{-1/4}\right)^3 dt$$

provided $T \ge C L^4(0)$

Pf of (****) is elementary. Here's a sketch:

<u>step 1</u>: View L as fn of E, not t. Then $(\dot{L})^2 \le C|\dot{E}|E$ becomes

$$\frac{1}{E}\left(\frac{dL}{de}\right)^2 |\dot{E}| \le C.$$

Thus for any fn $f(e)$,

$$C\int_0^T f(E(t))\,dt \ge \int_{E(T)}^{E(0)} \frac{f(e)}{e}\left(\frac{dL}{de}\right)^2 de.$$

step 2: Apply this to $f(e) = e^3$, getting

$$\int_{E(T)}^{E(0)} e^2 \left(\frac{dL}{de}\right)^2 de \le C \int_0^T E^3(t)\,dt.$$

Change vars on LHS to $\hat{e} = e^{-1}$

$$e^2 \left(\frac{dL}{de}\right)^2 de = -\left(\frac{dL}{d\hat{e}}\right)^2 d\hat{e}$$

so

$$\int_{E^{-1}(0)}^{E^{-1}(T)} \left(\frac{dL}{d\hat{e}}\right)^2 d\hat{e} \le C \int_0^T E^3(t)\,dt.$$

step 3: min of LHS is achieved when $L(\hat{e})$ is linear. This gives

$$\frac{|L(T) - L(0)|^2}{E^{-1}(T) - E^{-1}(0)} \le C \int_0^T E^3(t)\,dt$$

Suppose (for simplicity) $L(T) \ge 2L(0)$. Then we get

$$\int_0^T E^3(t)\,dt \ge L^2(T)\,E(T) \ge C\,E^{-1}(T).$$

So $h(T) = \int_0^T E^3\,dt$ has $h \ge C(\dot{h})^{-1/3}$. This easily gives $h \ge Ct^{1/4}$ for large t.

<u>step 4</u> Argt used $L(T) \geq 2L(0)$. If this fails, then L is rel small so E is rel. large. Easily dealt with separately.

What have we accomplished?

- Starting pt. was important

  - don't try to prove selfsimilarity
  - don't try to prove coarsening actually happens

since these assertions need a probabilistic view (+ perhaps they're not true). Instead, just show

  - coarsening can't take place faster than a rate set by dimensional analysis.

- Method was also important

  - two ways to measure local length scale, $E(t)$ + $L(t)$.

- interpolation ineq relates them
- energy ineq relates $\dot{L}$ + $\dot{E}$ (why? well, changing L requires motion. This should be assoc to decrease in E).

• Result obtained is fairly weak

- only a time-averaged bd! (can argt be improved to give a ptwise bd? Success would require extracting more info from pde)

Similar argts have been used on a handful of other problems, including these:

(1) "Mullins-Sekerka" evolution: two phases, as in this talk, but velocity law is nonlocal

V = jump in $\frac{\partial u}{\partial n}$ across Γ, where $\Delta u = 0$ in both phases, with $u = \kappa$ at Γ

Formal scaling is $\ell(t) \sim t^{1/3}$.
Time-averaged, 1-sided version proved by Kohn + Otto in original CMP paper

(2) Low-vol-fraction regime of Mullins-Sekerka.

When vol fr of one phase $\to 0$, dependence of "constant" in our isoper ineq. on vol fraction becomes important.

That, in turn, depends on the choice of neg norm!

Explored by Conti, Niethammer, Otto in recent SIAM J. Math Anal paper

(3) multicomponent versions of "motion by surface diff'n" + "Mullins-Sekerka" can be formulated. Bds extended to these by Kohn + Yan (Interfaces + Free Boundaries 2004)

(4) A rather different example: "epitaxial growth model"

$$u_t + \Delta^2 u + \operatorname{div}\left(2(1-|\nabla u|^2)\nabla u\right) = 0$$

ie steepest descent (in L^2) for

$$E = \int |\nabla\nabla u|^2 + (1-|\nabla u|^2)^2$$

This time choice of L is easy: just the L^2 norm of u.

But "interpoln ineq" is difficult (closely related to Aviles-Giga, to be discussed in Lecture 2). See Kohn + Yan (Commun Pure Appl Math 2004)

(5) coarsening of droplets, modeled by a 4th order "lubrication eqn"

$$h_t + \operatorname{div}\left(h\nabla\left(\Delta h - V'(h)\right)\right) = 0$$

which is assoc to $E = \int \frac{1}{2}|\nabla h|^2 + V(h)$ as "H^{-1} steepest descent with mobility h". See Otto, Rump, Slepcev (SIAM J Math Anal 2006) for (one-sided, time-averaged) coarsening bnds.

(6) Pego + Dai applied method to some mean field theories of coarsening; see Pego's lectures on coarsening + coagulation (CNA preprint 06-CNA-001) or Dai + Pego, SIAM J Math Anal 37 (2005)

(7) Esedoglu + Greer applied method to some discrete evolution eqns that "look like" finite-difference schemes for ill-posed diffusion. (Applns are in computer vision, and in aggregation models from biology). Requires discrete version of neg norms + interpoln ineq. See preprint on Esedoglu's website.

(8) steepest descents assoc some nonlocal energies were recently studied by Slepcev ("Coarsening in nonlocal interfacial systems", preprint)

Are there coarsening systems for which this method doesn't seem to work? Yes. One example: "2D grain growth" (plane is divided into grains, 120° angles at junctions, $V_{nor} = \kappa$, expect $l(t) \sim t^{1/2}$).

Still, the list of applns isn't bad, considering the simplicity of the idea.