Energy-Driven Pattern Formation

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Overview

What is energy-driven pattern formation? Some features:

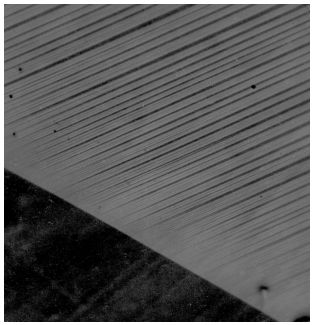
- Problems from physics, whose solutions involve microstructure
- Models from calculus of variations (nonconvex variational problems regularized by singular perturbations)
- Statics: energy scaling laws (at least the question makes sense)
- Dynamics: patterns induced by steepest-descent dynamics

Today: a few examples (not a survey).

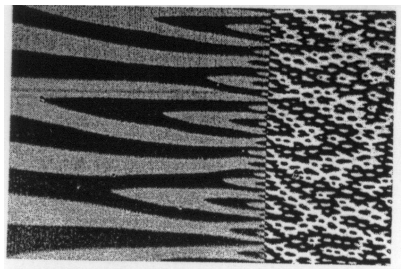
Statics

Pattern formation from energy minimization (some older examples):

Branching of twins near an interface between austenite and twinned martensite Figure: R. James. Theory: Kohn and Müller, CPAM, 1994.



Branching of magnetic domains in a uniaxial ferromagnet. Figure: Hubert and Schäfer. Theory: Choksi, Kohn, Otto, CMP, 1999.

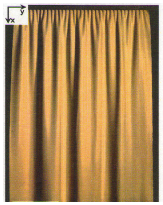


Vortices in type-II superconductors – the preferred arrangement seems to be a lattice (see eg work of Sandier & Serfaty).

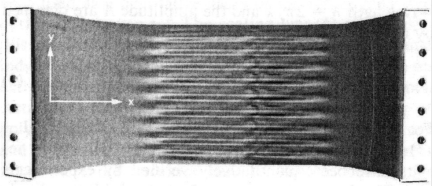
Wrinkling

A rich source of examples, where there has been recent progress: tension-driven wrinkling of thin elastic sheets

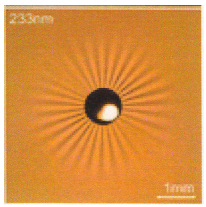
- hanging drapes (Vandeparre et al, PRL 2011)



- stretched sheets (Cerda & Mahadevan, PRL 2003)



- water drop on floating sheet (Huang et al, Science 2007)



Common features: Loading induces uniaxial tension. Wrinkles serve to avoid compression. Wrinkling direction is known. Scale of wrinkling may depend on location. Scale of wrinkling depends on sheet thickness.

Features shared by all these problems

- The physics is described by a nonconvex variational problem, regularized by higher-order term with a small parameter ε
- As $\varepsilon \to 0$, energy minimization requires microstructure. The effect of $\varepsilon > 0$ is to set the length scale (and perhaps to choose the pattern).

A basic 1D example with similar features:

$$\int_0^1 (u_x^2 - 1)^2 + \varepsilon^2 u_{xx}^2 + \alpha u^2$$

The 1D example

$$\int_0^1 (u_x^2 - 1)^2 + \varepsilon^2 u_{xx}^2 + \alpha u^2$$

(a) When $\varepsilon = 0, \alpha > 0$, min value is 0, not attained. Min sequence requires microstructure ("$u_x = \pm 1$, with prob $1/2$ each").

(b) When $\varepsilon > 0$, min scales like $\varepsilon^{2/3}\alpha^{1/3}$, since for a sawtooth with N teeth, value is approx $\varepsilon N + \alpha(1/N)^2$. Best $N \sim (\alpha/\varepsilon)^{1/3}$.

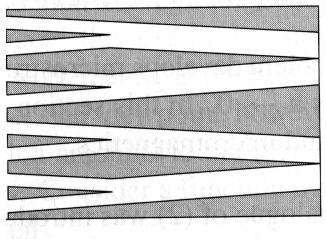
(c) The case $\varepsilon > 0, \alpha = 0$ is different: then there should be just one tooth, and the optimal value is $c_0\epsilon$.

(d) The optimal profile of a "tooth" (which determines c_0) can be found by minimizing $\int \varepsilon^{-1}(v^2 - 1)^2 + \varepsilon v_x^2$ among monotone v such that $v = -1$ for $x \ll 0$ and $v = 1$ for $x \gg 0$. Exactly solvable: $v = \tanh(x/\varepsilon)$.

Branching of twins

In 2D or 3D, emergence of microstructure may be due to the bdry conditions. Then microstructural length scale may vary with dist to bdry. Example modeling branching of twins (Kohn & Müller, 1994):

$$\min_{\substack{u_y=\pm 1 \\ u=0 \text{ at } x=0}} \int_0^1 \int_0^L u_x^2 + \varepsilon |u_{yy}| \, dx \, dy$$



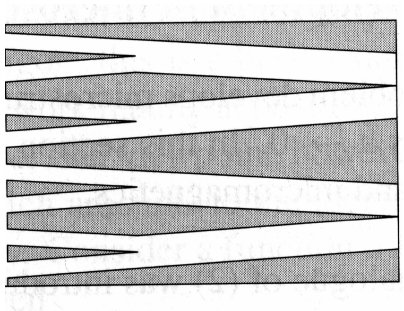
Simplified version of $\int_\Omega u_x^2 + (u_y^2 - 1)^2 + \varepsilon^2 |\nabla\nabla u|^2$. Essential character:

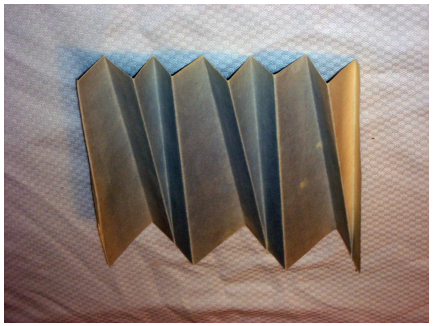
- "Bulk energy" prefers two possible slopes $\nabla u = (0, \pm 1)$.
- The boundary condition requires a fine-scale mixture.
- The singular perturbation ("surface energy") prefers fewer interfaces. But coarsening away from the edge costs energy ($u_x \neq 0$).

Branching of twins

$$\min_{\substack{u_y=\pm 1 \\ u=0 \text{ at } x=0}} \int_0^1 \int_0^L u_x^2 + \varepsilon |u_{yy}| \, dx \, dy$$

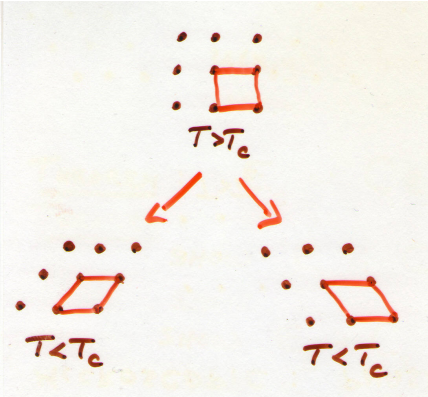
What happens? Length scale of twinning varies with distance to the boundary, $\ell(x) \sim \varepsilon^{1/3} x^{2/3}$. Schematic top view, photo showing mechanism of refinement, and actual twins:

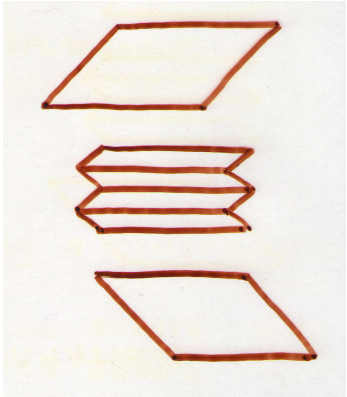




The underlying physics

Martensitic phase transformation: above T_c, atomic lattice is cubic; below T_c, period cell is a parallelogram: image of the cubic lattice under linear map $\begin{pmatrix} 1 & \pm a \\ 0 & 1 \end{pmatrix}$.





Variational problem is minimization of elastic + surface energy, if atom at (x, y) moves to $(x + au(x, y), y)$, and left hand boundary meets (rigid) austenite.

What can we hope to prove?

Fundamental difficulty: what is a pattern?

Proposal: Focus, for analysis, on identification of energy scaling law. (At least the question makes sense.) For the example at hand

$$\min_{\substack{u_y=\pm 1 \\ u=0 \text{ at } x=0}} \int_0^1 \int_0^L u_x^2 + \varepsilon |u_{yy}| \, dx \, dy$$

the main results are:

(a) Energy scaling law: $C\varepsilon^{2/3}L^{1/3} \leq \min \text{ energy} \leq C'\varepsilon^{2/3}L^{1/3}$.

(b) Local version: the energy in $[0, x] \times [0, 1]$ scales like $\varepsilon^{2/3}x^{1/3}$.

(c) Minimizer is self-similar near $x = 0$ [Conti, CPAM, 2000].

What kind of mathematics is needed? Focusing just on the energy scaling law $C\varepsilon^{2/3}L^{1/3} \leq \min \text{ energy} \leq C'\varepsilon^{2/3}L^{1/3}$:

- The upper bound is easy (sufft to find a good test function).
- The lower bound is more difficult (it must apply to any u).

The lower bound

$$\min_{\substack{u_y=\pm 1 \\ u=0 \text{ at } x=0}} \int_0^1 \int_0^L u_x^2 + \varepsilon |u_{yy}| \, dx \, dy \geq C\varepsilon^{2/3} L^{1/3}$$

Step 1: If the surface energy is large, we're done. If small, then at a generic x, the sawtooth $y \to u(x, y)$ has relatively few teeth.

Step 2: A sawtooth with few teeth and slopes ± 1 must make large excursions. Therefore the function $y \to u(x, y)$ has large L^2 norm.

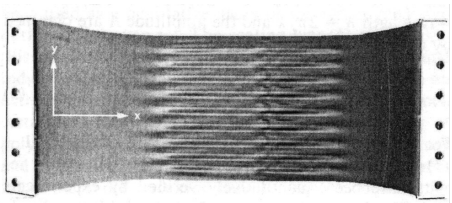
Step 3: Dropping the surface energy and the constraint $u_y = \pm 1$, the energy between 0 and x is bounded below by

$$\min_{\text{bndry conds}} \int_0^1 \int_0^L u_x^2 \, dx \, dy.$$

Easy to solve (convex!). The EL eqn is $u_{xx} = 0$. If $u = 0$ at LHS and L^2 norm is large at RHS, the value is large.

Remark: Essence of the argument: Step 2 amounts to interpolation between the BV, L^2, and H^{-1} norms of u_y); Step 3 uses the relaxation of the $\varepsilon = 0$ variational problem.

Returning to wrinkling



$$E_h = (\text{membrane energy}) \; + \; h^2(\text{bending energy}) + (\text{loads})$$

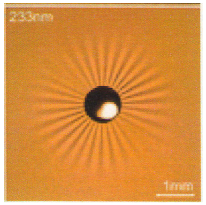
A calculus of variations problem involving configuration of the sheet, i.e. a map $u : \Omega \to R^3$, where $\Omega \subset R^2$ is the unloaded sheet.

The membrane energy prefers isometry; something like $\int_\Omega |Du^T Du - I|^2 \, dx$.

The bending energy penalizes curvature; something like $\int_{\text{image}} |\text{curvature}|^2 dx$. Prefactor is small: h is the sheet thickness.

Local minima of E_h are stable configurations. Since membrane energy is nonconvex and h is small, there should be many local minima. Do the configurations we see achieve (or approach) the global minimum?

The big picture



$$E_h = (\text{membrane energy}) \; + \; h^2(\text{bending energy}) + (\text{loads})$$

- If $h = 0$, minimization of membrane + loading terms requires infinitesimal wrinkling (and infinite bending energy). Analysis via "relaxed variational problem". Let $\mathcal{E}_0 = \min E_0$ be the min value when $h = 0$.
- When $h > 0$, competition between bending and membrane effects sets the local length scale of wrinkling. Let $\mathcal{E}_h = \min E_h$ be the min energy at fixed $h > 0$. Evidently

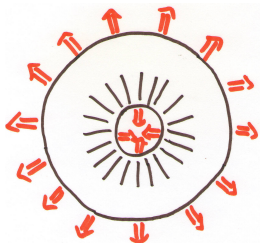
$$\mathcal{E}_h = \mathcal{E}_0 + \text{excess energy}.$$

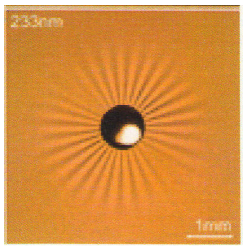
Convenient focus: identify the scaling law of the excess energy.

The annulus problem

Annulus-shaped sheet, loaded by uniform tension at both boundaries. Captures essential physics of the "drop on sheet" expt (cf Davidovitch et al, PNAS 2011).

No wrinkling at larger radii; lots of wrinkling at smaller radii, to avoid compression. Free boundary at $r = r_0$.





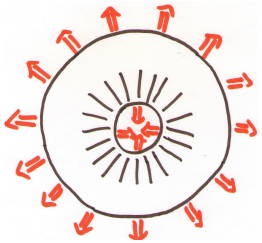
Studied with Peter Bella (CPAM 2014). Main conclusion: excess energy is linear in h,

$$\mathcal{E}_0 + C_1 h \leq \min E_h \leq \mathcal{E}_0 + C_2 h$$

Really two assertions:

- upper bound (requires a good ansatz)
- lower bound (ansatz-free!)

Key ideas



We use thin-sheet version of finite elasticity:

$$E_h = \int W_{\text{mem}}(Du) + h^2 \int |DDu_3|^2 + (\text{bdry terms assoc to loads})$$

where $u : R^2 \mapsto R^3$, u_3 is the out-of-plane deformation, and W_{mem} (derived from a 3D elastic energy) resembles $|Du^T Du - I|^2$.

Upper bound $\min E_h \leq \mathcal{E}_0 + Ch$ is not entirely trivial:

- Ansatz of form $u_3 = f(r)\sin(\theta/h^{1/2})$ doesn't quite work – it gives excess energy of order $h|\log h|$.
- One way to eliminate the logarithm: refine the scale of wrinkling repeatedly as $r \to r_0$. (Another way: keep length scale fixed as $r \to r_0$ but change the profile of the wrinkles.)

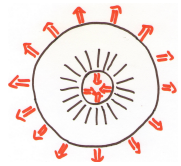
Key ideas, cont'd

Lower bound says $\min E_h \geq \mathcal{E}_0 + Ch$. Proof must be ansatz-free. Main steps:

Step 1 Soln of $h = 0$ ("relaxed") problem is infinitesimally wrinkled but planar. So out-of-plane deformation costs membrane energy. In particular, if a deformation u has excess energy less than δh, then

$$\int |u_3|^2 \leq C\delta h$$

(using only membrane effects).



Step 2 The excess energy includes all the bending energy. So if u has excess energy less than δh, then

$$\int |DDu_3|^2 \leq \delta h^{-1}.$$

Step 3 Use the interpolation inequality $\int |Df|^2 \leq (\int |f|^2)^{1/2} (\int |DDf|^2)^{1/2}$ with $f = u_3$ to see that

$$\int |Du_3|^2 \leq C\delta.$$

Step 4 So: if u has excess energy much smaller than h, then the associated deformation is (almost) planar and unwrinkled. But the min energy among unwrinkled planar deformations is much larger than $\mathcal{E}_0$, since no wrinkling $\Rightarrow$ compression in the hoop direction. So δ cannot be very small.

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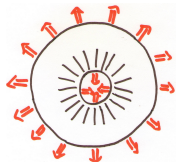

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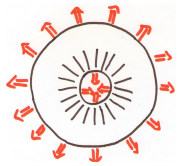

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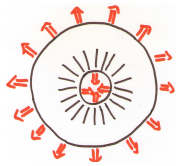

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There is more to life than statics

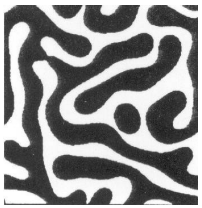
Focus thus far has been energy minimization, discussing just a couple of examples.

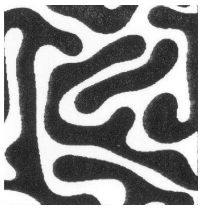
But nature is also full of transient patterns.

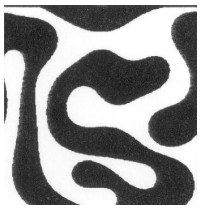
One class of examples: surface-energy-driven coarsening. Typical feature of coarsening: the system "forgets" its initial data, developing steady-state statistics (until finite-size effects set in).

Focus today: a bound on the coarsening rate for motion by surface diffusion (work with Felix Otto, CMP 2002). Key tools: interpolation inequalities (again!) and energy inequalities.

Coarsening


$t = 1$


$t = 2$


$t = 10$

Motion by surface diffusion: boundary $\Gamma(t)$ between two phases moves with normal velocity

$$v_{\text{nor}} = \Delta_\Gamma \kappa$$

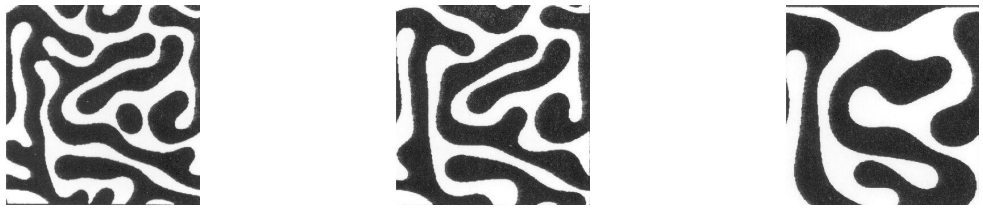
This evolution is energy-driven:

$$\frac{d}{dt}\text{Perimeter} = \int_\Gamma \kappa v_{\text{nor}} = -\int_\Gamma |\nabla_\Gamma \kappa|^2$$

Common belief, for random initial data:

- length scale coarsens, $\ell(t) \sim t^{1/4}$
- solution is statistically self-similar

Why is this difficult?



- Conjectured self-similarity might be wrong.

  Not even clear what it means!

- Assertion that $\ell(t) \sim t^{1/4}$ says

  (1) Solution never stops coarsening.
  False e.g. for spheres. Therefore subtle.

  (2) Solution doesn't coarsen faster.
  True without exception. Therefore accessible.

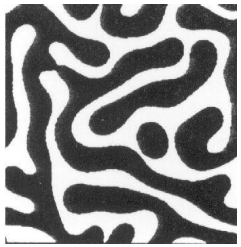
Analytic result: a weak version of (2), showing (very roughly)

$$\ell(t) \leq Ct^{1/4}$$

Two ways to measure local length scale

Represent structure by $\chi(x) = \pm 1$. Assume:

- spatially periodic (so averaging is easy)
- equal vol fractions (for simplicity only)

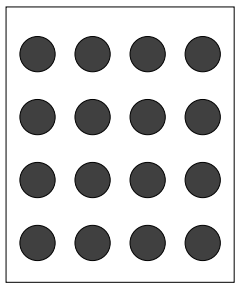


Our eye detects the length scale $\ell(t)$ easily. Two ways a computer could find it:

Method 1: E = perimeter per unit volume, scales like $1/\ell(t)$

Method 2: L = $\max_{|\nabla g| \le 1} \fint g\chi$, scales like $\ell(t)$

Consider periodic system with N inclusions and local length scale ℓ.



To see why $E \sim 1/\ell$, observe that $\frac{\text{perimeter}}{\text{area}} \sim \frac{N\ell}{N\ell^2}$.

To see why $L \sim \ell$, argue that best g has $g \sim \ell$ at inclusion centers, $g \sim -\ell$ far from inclusions, so $\chi g \sim \ell$.

Key observation

E and L are related by

- interpolation inequality: We always have

$$EL \geq \text{const.}$$

Proof makes no use of evolution law. Essentially:

$$\fint |\chi| \leq C \left(\fint |\nabla \chi|\right)^{1/2} \left(\fint |\nabla^{-1} \chi|\right)^{1/2}$$

- energy inequality: Solutions of the evolution law satisfy

$$dE/dt \leq 0 \quad \text{and} \quad (dL/dt)^2 \leq 2E|dE/dt|$$

Intuition why dE/dt controls dL/dt: coarsening requires motion, which dissipates energy. Proof is simple (like most energy inequalities).

These are sufficient (sort of)!

The available information

$$EL \geq C, \quad dE/dt \leq 0, \quad (dL/dt)^2 \leq 2E|dE/dt|$$

does not imply

$$L(t) \leq Ct^{1/4} \quad \text{or} \quad E(t) \geq Ct^{-1/4},$$

but it does imply a time-averaged version of the latter:

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

provided $T \gg L^4(0)$. Proof is an ODE argument (like Gronwall's inequality).

What is energy-driven pattern formation?

Today's examples were:

- Branching of twins
- Wrinkling of an elastic sheet
- Coarsening due to motion by surface diffusion

Some common themes:

- Questions from physics, posing challenges for analysis
- Energy-driven, but not necessarily at equilibrium
- Focus on examples; unity will emerge in due course.