R. Kohn – Lecture 4 (CMU): The Sharp-Interface Limit of Action Minimization.

Outline:

(1) What is "action minimization" + why is it interesting?

(2) Brief rmks about action minzn as a numerical problem

(3) Recent progress on sharp-interface limit of action minzn for Modica-Mortola

Related reading:

- my article in Proc ICM 2006 (close to parts (1) + (3) of above outline); also a short review by Maria Westdickenberg, "Rare events, action minimization, + sharp interface limits," available at her website www.math.gatech.edu/~maria/

- for followup on numerical action min, see recent article by Heymann + Vanden-Eijnden ("The geometric minimum action method...") avail from "early-view" part of Comm Pure Appl Math website; also, for "string methods" E, Ren, Vanden Eijnden, J Chem Phys 126 (2007) 164103

- for more abt sharp interface limit see Kohn - Reznikoff - Tonegawa, Calc Var PDE 25 (2006) 503-534; Tonegawa - Westdickenberg, Indiana Univ Math J 56 (2007) 2935-2990; Mugnai + Röger, Interfaces + Free Boundaries 10 (2008) 45-78.

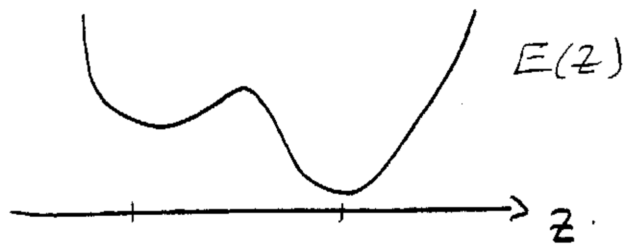
Starting pt: observe that nature finds local, not global, minima in many settings

- water can be heated > 100° C
- most foams are metastable (eg beer)
- crystals have defects

Energy-driven systems escape from local min via thermal fluctuations

- if deterministic dynamics is steepest descent for some energy ($\dot{z} = -\nabla E(z)$) then fluctuations are modelled via assoc stoch diff'l eqn $dz = -\nabla E\,dt + \text{noise}$

- small noise ⇒ escape from energy well is rare (but it happens eventually, with prob 1)

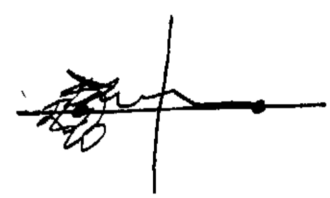


- events can be <u>rare</u> & yet <u>critically important</u> (eg failure of a computer's hard drive ...).

- many links to chemistry & physics (statistical physics of nucleation; timescale of crucial events such as protein folding; etc)

In finite dimensions there's a rather complete theory. Think eg of $E(z) = (z_1 - 1)^2 + z_2^2$

$$dz = -\nabla E(z)\,dt + \sqrt{2\delta}\,dW$$



Transitions are rare, yet predictable. In particular:

<u>Large Deviation Principle</u>: Given that transition takes time $\leq T$, it occurs (with overwhelmingly high prob) by approx the pathway that minimizes the <u>action fnl</u>

$$S_T = \min_{\substack{z(0)=(-1,0)\\ z(T)=(+1,0)}} \frac{1}{4}\int |\dot{z} + \nabla E|^2\,dt$$

Also,

$$\text{Prob}(\text{Switch by time } T) \sim C e^{-S_T/\varepsilon}$$

Notes:

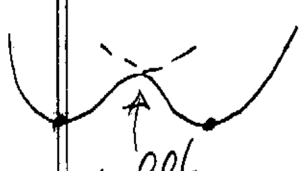
a) not limited to gradient systems; for $dz = f(z)\,dt + \sqrt{2\varepsilon}\,dw$, action is $\int |\dot z - f(z)|^2\,dt$. Integrand is always "eqn error".

b) see book by Freidlin + Wentzell for comprehensive treatment; for a fairly elementary appln involving magnetic switching see Kohn - Reznikoff - Vanden-Eijnden J Nonlin Sci 15 (2005) 223 - 253.

c) for gradient systems, as $T \to \infty$, action-min path is easy to describe:

- it starts by going "directly uphill" to lowest mtn pass; then
- it continues by going "directly downhill from mtn pass"

To see this: let τ = time of arrival at ridge



$$\frac{1}{4}\int_0^\tau |\dot z + \nabla E|^2 = \underbrace{\frac{1}{4}\int_0^\tau |\dot z - \nabla E|^2}_{\geq 0} + \underbrace{\int_0^\tau \langle \dot z, \nabla E\rangle}_{E(\tau) - E(0)}$$

so Action $\geq$ E(mtn pass) − E(initial state).

If T is large enough, we can (almost) achieve equality by setting $\dot{z} = \nabla E$ until we reach saddle. (T must be large since $\dot{z} = \nabla E$ takes inf time to arrive at saddle.)

d) for T fixed, soln is different (saddle may be irrelevant). Recall: fixing T is natural. (Early failures, though extremely rare, may be the ones we care about most.)

<u>What are the math problems here?</u>

<u>Problem 1</u>: Find mtn pass (lowest-energy saddle pt) numerically.

Relevant to large-T limit, for gradient systems.

Conceptually simple ("mtn pass lemma" has been used for proving existence of saddle pts for decades). But not so trivial to implement numerically, if E is only accessible numerically.

Numerical schemes mainly invented/studied by chemists! Best, until recently, was "nudged elastic band method."

Recent progress: "string method" (E, Ren, Vanden Eijnden) is more or less an improved implementation of "mtn pass lemma".

Problem 2: Find min action path, in settings where finding saddle pt's isn't suff't (non-gradient system, or finite T).

Direct discretization of defn has been done, but works poorly since tie-parzn is very uneven.

Better: decouple spatial path from its parzn in time. Pbm of finding opt'l path can be reduced to something very similar to finding geodesics in a Riemannian metric. (See recent work of Heymann + Vanden Eijnden).

Problem 3: What happens when energy is infinite-dimensional, for example "Modica - Mortola"?

Focus for rest of this lecture on Pbm 3: action minzn for

$$(*) \qquad E_\varepsilon = \int_\Omega \frac{\varepsilon}{2}|\nabla u|^2 + \frac{1}{4\varepsilon}(u^2-1)^2$$

Warming up:

A) "steepest descent" for (*) is "Allen-Cahn eqn"

$$\dot{u} - \varepsilon \Delta u + \frac{1}{\varepsilon}(u^3-u) = 0.$$

So "noisy steepest descent" is a stochastic pde. Hard to interpret. But there's no problem with the action fnl. – it's just the integral of eqn error.

B) Limit $\varepsilon \to 0$ corresponds to considering the fixed energy $\int \frac{1}{2}|\nabla u|^2 + \frac{1}{4}(u^2-1)^2\, dx$ on larger + larger domains; for example in 1D (with $y = x/L$)

$$\int_0^L \frac{1}{2} u_x^2 + \frac{1}{4}(u^2-1)^2\, dx = \int_0^1 \frac{1}{2L} u_y^2 + \frac{L}{4}(u^2-1)^2\, dy$$

thus $\frac{1}{L} = \frac{\text{(scale on which } u \text{ changes)}}{\text{(scale of domain)}}$ plays role of ε.

c) Limit of Allen-Cahn as $\varepsilon \to 0$ is motion by curvature on timescale $1/\varepsilon$ (in dim ≥ 2). So it's natural to rescale time in such a way that u_ε evolves on timescale of order 1. Therefore we work with

$$\varepsilon u_t = \varepsilon \Delta u - \frac{1}{\varepsilon}(u^3 - u)$$

and action min becomes

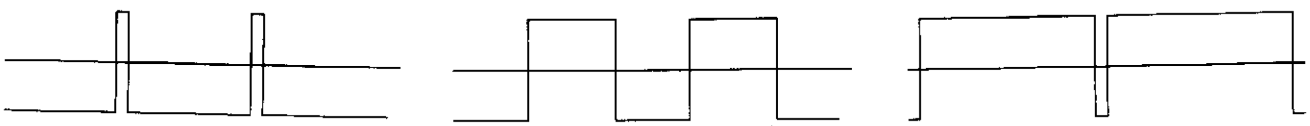
$$\min_{\substack{u \equiv -1 \text{ at } t=0 \\ u \equiv +1 \text{ at } t=T}} \frac{1}{4} \int_0^T \int_\Omega \left| \varepsilon^{1/2} u_t - \varepsilon^{-1/2}\left(\varepsilon \Delta u - \varepsilon^{-1}(u^3 - u)\right) \right|^2 dx\,dt$$

$$\frac{1}{4} \iint \left| \varepsilon^{1/2} u_t + \varepsilon^{-1/2} \nabla E_\varepsilon \right|^2$$

D) if Ω is convex (or using periodic bc), $u \equiv +1$ and $u \equiv -1$ are the <u>only</u> local min of E_ε (the energy landscape is relatively simple!).

Question: what do action minimizers look like as $\varepsilon \to 0$?

1D periodic answer (fully rigorous - see Kohn-Reznikoff-Tonegawa Calc Var PDE paper): system "nucleates" N seeds (2N walls), equispaced; they then propagate at const. velocity. Opt'l value of N depends on T.



$t \approx 0$ $\qquad$ $t = T/2$ $\qquad$ $t \approx T$

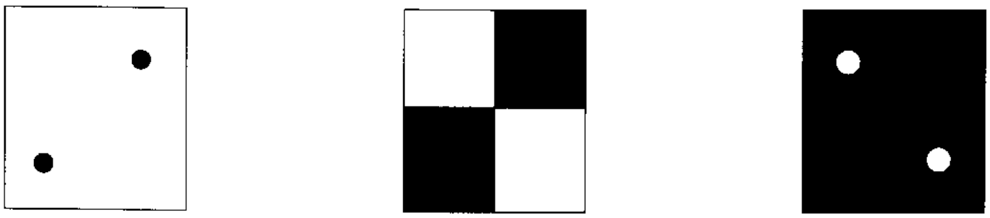
2D answer (sharp interface limit was justified by Mugnai + Röger IFB paper; figure below is just a guess of the optimal path when T is fairly large; see E, Ren, VandenEijnden, CPAM 57 (2004) 637-656 for 2D numerics):

Like 1D, except that

a) "nucleation" of seeds can be cost-free, if seeds start as pts (so perimeter = 0)

b) "propagation" can be cost-free when surface moves with velocity = -curvature

One possible pathway:



$t \approx 0$ $\quad$ $t = T/2$ $\quad$ $t \approx T$

Best pathway solves var'l pbm

$$\min_{\text{pathways}} \{\text{nucl cost, if any}\} + \int_0^T \int_{\Gamma(t)} (V_{nor}+K)^2$$

eqn error
assoc w/ motion
by curvature

Rmk: analysis of sharp-interface limit in 2D (and 3D) is closely connected to a conjecture of De Giorgi that (roughly speaking)

$$\int_\Omega \varepsilon^{-1} |\nabla E_\varepsilon|^2 \xrightarrow[\Gamma]{} \int_{\text{interface}} (\text{curvature})^2 .$$

(Recently proved by Röger + Schätzle in 2D + 3D.)

Some basic ingredients of rigorous analysis:

(1) <u>Jumps in energy cost action</u>. (Thus, for example, in 1D nucl of any seed costs action.)

<u>Pf</u>: $\frac{1}{4}\int_{t_1}^{t_2}\int_\Omega |\varepsilon^{1/2} u_t + \varepsilon^{-1/2}\nabla E_\varepsilon|^2 = \frac{1}{4}\int_{t_1}^{t_2}\int |\varepsilon^{-1/2} u_t - \varepsilon^{-1/2}\nabla E_\varepsilon|^2$

$$+ \int_{t_1}^{t_2} \langle u_t, \nabla E_\varepsilon \rangle$$

$$\geq E(t_2) - E(t_1)$$

(familiar argt!)

(2) <u>Action controls wall profile + velocity</u>

In fact, $S_T \geq \frac{1}{4}\int_0^T\int_\Omega \varepsilon u_t^2 + \varepsilon^{-1}|\nabla E_\varepsilon|^2$

since $E = 0$ when $u \equiv -1$ and $u \equiv +1$, and using fact that

$$S_T = \frac{1}{4}\int_0^T\int_\Omega \varepsilon u_t^2 + \varepsilon^{-1}|\nabla E_\varepsilon|^2 + 2\langle u_t, \nabla E_\varepsilon \rangle$$

this term integrates to $E(T) - E(0) = 0$,

(3) <u>Propagation cost is of order 1.</u> In fact

$$\frac{4}{3}|\Omega| = \int_0^T \int_\Omega u_t (1-u^2)\, dx\, dt$$

$$\le \left(\iint \varepsilon u_t^2\right)^{1/2} \left(\iint \varepsilon^{-1} (u^2-1)^2\right)^{1/2}$$

we'll relate this soon to "prop cost"

not too large (controlled by energy).

Here's a nontechnical pass at 1D analysis (captures most of main ideas while avoiding many technicalities). Suppose we accept that

a) all nucleations occur at $t=0$ and all annihilations occur at $t=T$.

b) energy is "equipartitioned," ie

$$\int \frac{\varepsilon}{2} |u_x|^2\, dx = \int \frac{1}{4\varepsilon} (u^2-1)^2\, dx = \frac{1}{2} E$$

at each time t, $0<t<T$.

Then we can show the (optimal!) lower bd (using $\Omega = [0,L]$ with periodic bc)

$$(\ddagger\ddagger) \quad \text{min action} = \min_{N \geq 1} \left\{ 2Nc_0 + \frac{L^2}{9TNc_0} \right\}$$

with $c_0 = 2\frac{\sqrt{2}}{3}$ = energy of one wall
(so 1st term = "nucl cost" and 2nd = "prop. cost").

Step 1: $\frac{4}{3}L \leq \left(\iint \varepsilon u_t^2\right)^{1/2}\left(\iint \varepsilon^{-1}(1-u^2)^2\right)^{1/2}$. same as item ③ above.

Step 2: $\int_0^T\int_0^L \varepsilon^{-1}(1-u^2)^2 = \int_0^T 2E = 4c_0NT$ if N nuclei form (making $2N$ walls)

using hypoth (a) + (b) & supposing each wall has minimal energy

Step 3: $\frac{1}{4}\int_\delta^{T-\delta}\int \varepsilon u_t^2 \leq \frac{1}{4}\int_\delta^{T-\delta}\int \varepsilon u_t^2 + \varepsilon^{-1}|\nabla E_\varepsilon|^2$ (trivial)

$$= \underbrace{\frac{1}{4}\int_\delta^{T-\delta}\int |\varepsilon^{1/2}u_t + \varepsilon^{-1/2}\nabla E_\varepsilon|^2}_{\substack{\text{"propagation cost"} \\ \text{portion of action,} \\ \text{by defn + hypoth (a),}}} \quad \text{hypoth (a),}$$

Collecting:

action assoc $0 < t < \delta \geq 2 N c_0$ if N seeds form, by pt ① and hypoth (a)

action assoc $\delta < t < T - \delta \geq \dfrac{\frac{1}{4}\left(\frac{4}{3}L\right)^2}{4 c_0 N T}$ by combining steps 1, 2, 3.

Adding these gives (**).

Remaining ingredients of 1D rigorous analysis are:

- pf that energy jumps only at discrete times, by amt assoc creation or annihilation of walls
- pf that away from these special times energy is indeed "equipartitioned"
- argt similar to above, but localized in space + time so no hypoth is needed abt when walls nucleate or annihilate.

For more, see the articles cited.

Stepping back: we've seen

- action minz'n is relevant
- numerical analysis is very underdeveloped, even in low dimensions
- sharp-interface limit shares features with static Modica-Mortola, but it's different because we're studying action-min <u>pathways</u> (evolving fronts!)