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

Outline:

1. What is "action minimization" & why is it interesting?

2. Brief remarks about action minimization as a numerical problem

3. Recent progress on sharp-interface limit of action minimization for Modica-Mortola

Related reading:

- my article in Proc ICM 2006 (close to parts (1) & (2) 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 more abt sharp interface limit see

Starting pt. is observe that nature finds

local, not global, minima in many settings

- water can be heated $> 100^\circ C$
- 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 stock diff eqn $\dot{z} = -\nabla E dt + \text{noise}$

- small noise $\Rightarrow$ escape from energy well is rare (but it happens eventually, with prob 1)
- events can be rare yet critically important (e.g., failure of a computer's hard drive ...).

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

\[ E(\tau) = (\tau - 1)^2 + \tau^2 \]

\[ d\tau = -\sqrt{E(\tau)} dt + \sqrt{2\theta} dW \]

Transitions are rare, yet predictable. In particular:

**Large Deviation Principle**: Given that transition takes time \( < T \), it occurs (with overwhelmingly high prob) by approx. the pathway that minimizes the action

\[ S_T = \min_{\tau(0) = (-1, 0), \tau(T) = (1, 0)} \int_0^T \left( \frac{1}{2} \dot{\tau}^2 + 2E\tau^2 \right) dt \]
Also,

\[
\text{Prob (Switch by time } T) \sim C e^{-S/T}
\]

Notes:

a) not limited to gradient systems; for
\[d\hat{z} = f(z) dt + \sqrt{2b} dW,\]
action is \[\int_0^T \frac{1}{2} - f(z)^2 \, dt,\]
intergrand is always "eqn error".

b) see book by Franklin + Wertz for comprehensive treatment; for a fairly
elementary app in involving magnetic switching, see Kohl - Reznikoff - Verble - Epstien.

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

- it starts by going "directly uphill" to
least min pass; then

- it continues by going "directly
downhill from min pass"

To see this: let \( t = \) time of arrival at ridge

\[
\frac{1}{4} \int_0^T \dot{z}^2 + VE^2 = \frac{1}{4} \int_0^T \dot{z}^2 - VE^2 + \int_0^T \frac{\dot{z} \cdot \dot{V} E}{E(t) - E(0)}
\]
So \[ \text{Action} \geq E(\text{mtn pass}) - E(\text{initial state}). \]

If \( T \) is large enough, we can (almost) achieve equality by setting \( \dot{z} = 7E \) until we reach saddle? (\( T \) must be large since \( \dot{z} = 7E \) takes out time to arrive at saddle.)

\( d) \) for \( T \) fixed, \( \dot{z} \rightarrow 0 \) is different (saddle may be irrelevant). Recall \( \dot{z} \) fixed \( T \) is natural. (Early failures, though extremely rare, may be the ones we care about most.)

What are the worst problems here?

**Problem 1**: 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) in more or less an improved implementation of "with pass lemma."

Problem 2: Find min action path, in settings where finding saddle pts can't suffice (non-gradient system, or finite $T$).

Direct discretization of above has been done, but works poorly since tri-pars is very uneven.

Better: decouple spatial path from its pars in time. Problem of finding optimal 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 "Hodler-Mantle"?

Focus for rest of this lecture on Problem 3: action minmization for

\[ E_\varepsilon = \int \frac{\varepsilon}{2} \dot{u}^2 + \frac{1}{4\varepsilon} (u^2 - 1)^2 \]

Warming up:

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

\[ \dot{u} = \varepsilon \Delta u + \frac{1}{\varepsilon} (u^2 - u) = 0. \]

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

B) Limit \( \varepsilon \to 0 \) corresponds to considering the fixed energy \( \int \frac{1}{2} \dot{u}^2 + \frac{1}{4} (u^2 - 1)^2 \) dx on larger and larger domains; for example in 1D (with \( y = \sqrt{\varepsilon} \))

\[ \int_0^L \frac{1}{2} u_x^2 + \frac{1}{4} (u^2 - 1)^2 \, dx = \int_0^1 \frac{1}{2L} u_y^2 + \frac{1}{4} (u^2 - 1)^2 \, dy \]
thus \( \frac{1}{L} = \frac{\text{scale on which \( \varepsilon \) changes}}{\text{scale of domain}} \) plays role of \( \varepsilon \).

C) Limit of Allen-Cahn as \( \varepsilon \to 0 \) is written by curvature on timescale \( \varepsilon \) (in dim \( \geq 2 \)). So it's natural to rescale time \( t \) in such a way that \( \varepsilon \) evolves on the scale of order 1. Therefore we work with

\[ \varepsilon u_t = \varepsilon du - \frac{1}{\varepsilon}(\varepsilon^2 u - u) \]

and action \( \text{min} \) becomes

\[ \text{min} \int_0^T \frac{1}{4} \left( \frac{1}{\varepsilon} u_t^2 - \varepsilon^{-\frac{1}{2}} (\varepsilon du - \varepsilon^{-1}(\varepsilon^2 u - u))^2 \right) dx \]

\[ u = -1 \text{ at } t = 0 \]
\[ u = +1 \text{ at } t = T \]

\[ \frac{1}{4} \int \left( \varepsilon^{\frac{1}{2}} u_t + \varepsilon^{-\frac{1}{2}} \nabla \varepsilon \right)^2 \]

D) if \( \Omega \) is convex (or using periodic bc), \( u = 1 \) and \( u = -1 \) are the only local min of \( \mathcal{E}_\varepsilon \) (the energy landscape is relatively simple!).

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Question: What do action minimizers look like as \( \varepsilon \to 0 \)?
1D periodic answer (fully rigorous - see Kohn-Regnikoff-Tongawa Calc Var PDE paper) is system "nucleates" N seeds (2N wells), equispaced; they then propagate at const. velocity. Optimal value of N depends on T.

\[ \begin{array}{cccc}
\text{t = 0} & \text{t = T/2} & \text{t = T}
\end{array} \]

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

Like 1D, except that

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

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

$t = 0$

$t = T/2$

$t = T$

Best pathway solves variational problem:

\[
\min \left\{ \text{nucleation cost, if any} \right\} + \int_0^T (V_{\text{curvature}}) \, dt
\]

\[\Gamma(t)\] is given error associate motion by curvature.

Rigorous analysis of sharp-interface limit, in 2D (and 3D) is closely connected to a conjecture of De Giorgi. That (roughly speaking)\n
\[
\int_{\Omega} E^{-1/2} \left| J \right| E_c \, dx \rightarrow \int_{\text{interface}} \left( \text{curvature} \right)^2
\]

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

Some basic ingredients of rigorous analysis:
(1) \textbf{Jumps in energy cost action.} (Thus, for example, in 1D, much of any small costs action.)

\[ \frac{1}{4} \int_{t_1}^{t_2} \left( E \epsilon u_t + \epsilon^{-1} |\nabla E \epsilon| \right)^2 dt \]

\[ \geq E(t_2) - E(t_1) \]

(familiar arg!)

(2) \textbf{Action controls well profile + velocity.}

In fact,

\[ S_T = \frac{1}{4} \int_0^T \int \left( E u_t^2 + \epsilon^{-1} |\nabla E \epsilon| \right) dt \]

since \( E = 0 \) when \( u = -1 \) and \( u = +1 \), and using fact that

\[ S_T = \frac{1}{4} \int_0^T \int \left( E u_t^2 + \epsilon^{-1} |\nabla E \epsilon|^2 + 2 \langle u_t, \nabla E \epsilon \rangle \right) dt \]

this term integrates to

\[ E(t) - E(0) = 0 \]
Propagation cost is of order 1. In fact

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

\[
\leq \left( \int \sum \varepsilon u_t^2 \right)^{1/2} \left( \int \sum \varepsilon^{-1} (u^2 - 1)^2 \right)^{1/2}
\]

We'll relate this soon to "prop cost not too large (controlled by energy)."

Here's a non-technical 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," i.e.

\[
\int \frac{3}{2} |u_t|^2 \, dx = \int \frac{1}{4E} (u^2 - 1)^2 \, dx = \frac{1}{2} E
\]

at each time \( t \), \( 0 \leq t \leq T \).

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

$$\text{min action} = \min_{N \geq 1} \left\{ 2 N c_0 + \frac{L^2}{97Nc_0} \right\}$$

with $c_0 = 2 \frac{\sqrt{2}}{3} = \text{energy of one well}$

(so 1st term = "nuclei cost" and 2nd = "prop. cost")

Step 1: $\frac{4}{3} L \leq (\frac{1}{2} \sum_{k} \bar{E}_k^2)^{\frac{1}{2}} (\sum_{k} (1 - \bar{u}_k^2)^\frac{1}{2}$. same as item 3 above.

Step 2: $\int_{0}^{L} \int_{0}^{T} \bar{E}^{-1} (1 - \bar{u}_k^2) = \int_{0}^{T} 2 \bar{E} = 4 c_0 N T$ if $N$ nuclei form (making $2N$ wells)

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

Step 3: $\frac{1}{4} \int_{\frac{T}{8}}^{T-\frac{5}{8}} \frac{1}{2} \sum_{k} \bar{E}_k^2 \leq \frac{1}{4} \int_{\frac{T}{8}}^{T-\frac{5}{8}} \bar{E}_k^2 + \bar{E}_0 \left| \nabla \bar{E}_0 \right|^2$ (trivial) hypoth (a),

$$= \frac{1}{4} \int_{\frac{T}{8}}^{T-\frac{5}{8}} \left[ \bar{E}_k^2 + \bar{E}_0 \left| \nabla \bar{E}_0 \right|^2 \right]$$

"propagation cost"

portion of action, by data + hypoth (a),
Collecting:

action assoc \( 0 < t < \delta \geq 2Nc_0 \), if \( N \) seeds form, by pt 0 and hypoth (a)

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

Adding these gives (***),

Remaining ingredients of 1D rigorous analysis are:

- pt that energy jumps only at discrete times, by ampt assoc creation or annihilation of wells

- pt that away from these special times, energy is indeed "equipartitioned"

- ampt similar to above, but localized in space + time so no hypoth is needed alt when wells nucleate or annihilate.

For more, see the articles cited.
Stepping back: we've seen

- action minima are 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 pathways (evolving fronts!)