A model of rate-independent droplet evolution

Will Feldman

University of Utah

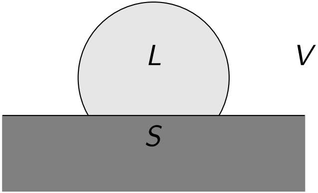
based on joint works with Inwon Kim (UCLA) and Norbert Požár (Kanazawa),

and with Carson Collins (UCLA)

Research supported by NSF grant DMS-2407235

Capillary energy

Configuration of solid liquid and vapor (air), subsets of $\mathbb{R}^{d+1} = \mathbb{R}^3$:



Given distinct phases $A, B \in \{S, L, V\}$ define the two-phase interface

$$\Sigma_{AB} = \partial A \cap \partial B \quad \text{with associated energy density} \quad \gamma_{AB}$$

Total interfacial energy – ignoring volume forces e.g. gravity –

$$E = \gamma_{SL}|\Sigma_{SL}| + \gamma_{SV}|\Sigma_{SV}| + \gamma_{LV}|\Sigma_{LV}|.$$

Disclaimer: energy computed inside of some bounded container

Capillary energy: PDE conditions

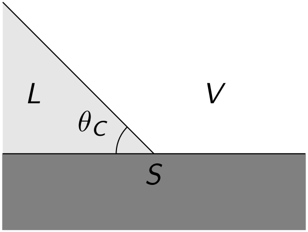
Total interfacial energy

$$E = \gamma_{SL}|\Sigma_{SL}| + \gamma_{SV}|\Sigma_{SV}| + \gamma_{LV}|\Sigma_{LV}|.$$

First variation (with volume constraint) gives PDE conditions

$$\begin{cases} 2\gamma_{LV}\kappa_{LV} = p & \text{on } \Sigma_{LV} \cap S^{\complement} \\ \cos\theta_C = \dfrac{\gamma_{SV} - \gamma_{SL}}{\gamma_{LV}} & \text{on } \Gamma := \partial S \cap \partial L \cap \partial V \end{cases}$$

contact angle θ_C along contact line Γ equals the *Young angle* defined by $\cos\theta_Y := \frac{\gamma_{SV} - \gamma_{SL}}{\gamma_{LV}}$. Pressure p is Lagrange multiplier for volume constraint, κ_{LV} is mean curvature.



Re-normalization

Since $\Sigma_{SL} \cup \Sigma_{SV} = \partial S$ we can, up to changing energy by an additive constant, consider instead

$$E_1 = \gamma_{LV}|\Sigma_{LV}| + (\gamma_{SL} - \gamma_{SV})|\Sigma_{SL}|.$$

By dividing through by γ_{LV} we can reduce to

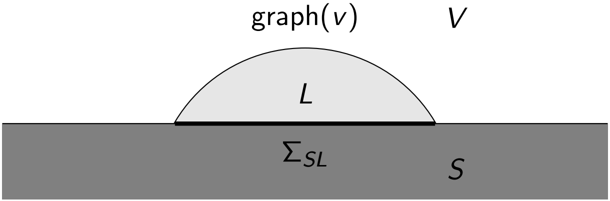
$$E_2 = |\Sigma_{LV}| - \cos\theta_Y |\Sigma_{SL}|$$

where, again, $\cos\theta_Y := \frac{\gamma_{SV}-\gamma_{SL}}{\gamma_{LV}}$ is the *Young contact angle*.

A (partially) linearized model

In the regime of small contact angle and subgraphical liquid region the capillary energy (partially) linearizes to another classic free boundary model. The main results of the talk discussed later will be for this (partially) linearized model.

Specifically, in this scenario, $L = \{0 \leq z \leq v(x)\}$ for some $v : \mathbb{R}^2 \to [0, \infty)$. Note wetted set $\Sigma_{SL} = \{v > 0\}$.



$$E = \int_{\Sigma_{SL}} \sqrt{1 + |\nabla v|^2} - \cos \theta_Y \, d\mathcal{H}^2(x)$$

A partially linearized model

In the regime of small contact angle and subgraphical liquid region the capillary energy linearizes to another classic free boundary model. Rescaling $v(x) = (\tan\theta_Y)u(x)$

$$
\begin{aligned}
E &= \int_{\Sigma_{SL}} \sqrt{1+\tan^2\theta_Y|\nabla u|^2} - \cos\theta_Y \; dx \\
&\approx \int_{\Sigma_{SL}} 1 + \frac{1}{2}\tan^2\theta_Y|\nabla u|^2 - \cos\theta_Y \; dx \\
&= \frac{1}{2}\tan^2\theta_Y \left[\int_{\{u>0\}} |\nabla u|^2 + 2\frac{(1-\cos\theta_Y)}{\tan^2\theta_Y} \; dx \right]
\end{aligned}
$$

Energy in brackets is known as *Alt-Caffarelli one-phase functional*.

A partially linearized model

Alt-Caffarelli one-phase energy functional

$$\mathcal{J}(u) = \int |\nabla u|^2 + Q^2 \mathbf{1}_{\{u>0\}} \, dx.$$

First variation gives a free boundary problem analogous to the capillary problem, called the *Bernoulli one-phase problem*,

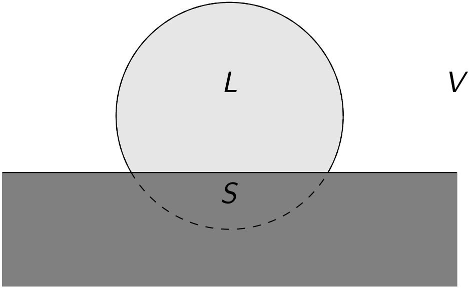
$$\begin{cases} -\Delta u = p & \text{in } \{u > 0\} \\ |\nabla u| = Q & \text{on } \partial\{u > 0\}. \end{cases}$$

Pressure $p > 0$ is Lagrange multiplier for volume constraint or 0 if we solve a Dirichlet problem instead.

Disclaimer: usually we are in a bounded container.

Classical capillary model: drops sitting on a flat surface

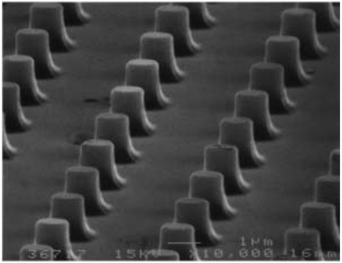
Only constant mean curvature surfaces with constant contact angle to a planar surface are *spherical caps*. Even adding gravity the shape is guaranteed to be axisymmetric.

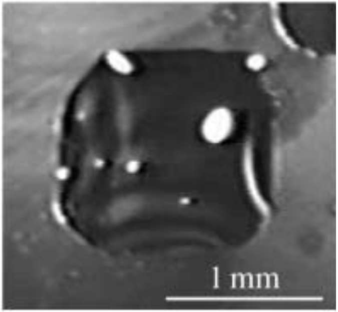


Drops even on quite smooth surfaces often don't look like this.

[Wente '80]

Liquid drops on rough surfaces





Marzolin, Smith, Prentiss and Whitesides *Adv. Mater.* (1998)
Bico, Tordeaux and Quéré *Euro. Phys. Lett.* (2001)

Liquid drops on rough surface

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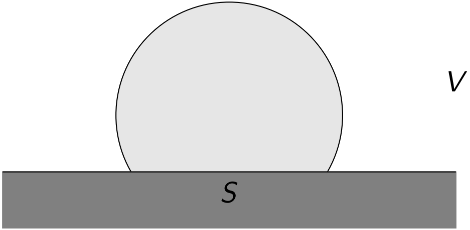
Empirical discussion of pinning

Slow condensation / evaporation or other slow volume forcing. Contact line only moves inwards below the receding angle θ_{rec}, only moves outward above the advancing angle θ_{adv}. There are known as the *dynamic contact angles*. Here consider $\theta_{rec} = \frac{\pi}{2}$ in an evaporating drop:



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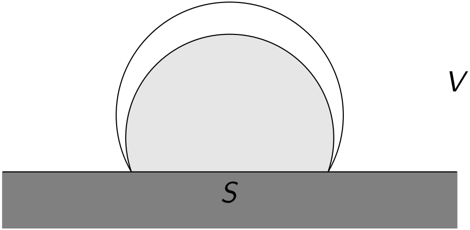

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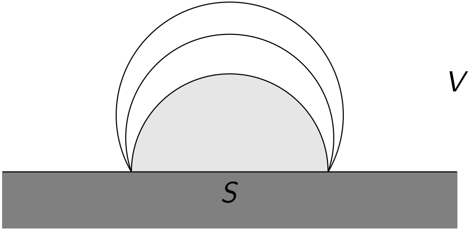

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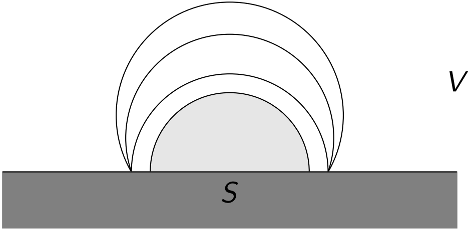

Energy and dissipation

Alt-Caffarelli energy functional

$$\mathcal{J}(u) = \int_U |\nabla u|^2 + \mathbf{1}_{\{u>0\}} \, dx, \tag{1}$$

augmented with a *dissipation distance* which (in concept) measures the energy dissipated due to static friction as the wetted region moves from Ω_0 to Ω_1

$$\mathrm{Diss}(\Omega_0, \Omega_1) = \mu_+|\Omega_1 \setminus \Omega_0| + \mu_-|\Omega_0 \setminus \Omega_1|,$$

or write $\mathrm{Diss}(u, v) = \mathrm{Diss}(\{u > 0\}, \{v > 0\})$.

The coefficients $\mu_+ > 0$ and $\mu_- \in (0, 1)$ can be viewed as the friction forces per unit length of the contact line, respectively for advancing and receding regimes.

Dirichlet driven quasi-static evolution

The evolution of the state $u(t) \in H^1(U)$ we consider is built on the following hypotheses (first stated vaguely)

1. (*Forcing*) External forcing drives the system to evolve: e.g. Dirichlet forcing on ∂U (our case) or varying volume constraint.
2. (*Local equilibrium*) The time-scale of the variations in the forcing is sufficiently slow that we can assume the system is always in local equilibrium (balance of surface tensions and frictional forces).
3. (*Frictional dissipation*) The energy dissipated due to friction on an infinitesimal variation is determined by the dissipation rate functional

$$\begin{aligned}\mathcal{R}(\Omega(0), V) &:= \int_{\partial\Omega(0)} \mu_+(V_n)_+ + \mu_-(V_n)_- \, dS \\ &= \frac{d}{dt}\bigg|_{t=0} \mathrm{Diss}(\Omega(0), \Omega(t))\end{aligned}$$

Energy solutions

Definition

A measurable $u : [0, T] \to H^1(U)$ is a *energy solution* (E) if:

1. (*Forcing*) For all $t \in [0, T]$: $u(t) = F(t)$ on ∂U.
2. (*Global stability*) The solution $u(t) \in H^1(U)$ and satisfies for all $t \in [0, T]$:

   $$\mathcal{J}(u(t)) \leq \mathcal{J}(u') + \mathrm{Diss}(u(t), u') \qquad \text{for all } u' \in u(t) + H^1_0(U).$$

3. (*Energy dissipation inequality*) For every $0 \leq t_0 \leq t_1 \leq T$ it holds

   $$\mathcal{J}(u(t_0)) - \mathcal{J}(u(t_1)) + \int_{t_0}^{t_1} 2\dot{F}(t)P(t)\, dt \geq \mathrm{Diss}(u(t_0), u(t_1)).$$

   Here $P(t) = P(u(t)) = \int_{\partial U} \frac{\partial u(t)}{\partial n}\, dS$ is an associated pressure.

[DeSimone-Grunewald-Otto] and [Alberti-DeSimone]

Time incremental / minimizing movements scheme

A very natural way to generate energy solutions is by a time incremental / minimizing movements evolution

$$u_\delta^k \in \operatorname{argmin}\left\{\mathcal{J}(w) + \operatorname{Diss}(u_\delta^{k-1}, w) : w \in F(k\delta) + H_0^1(U)\right\}.$$

Or, in more detail,

1. Given current state u_δ^{k-1}
2. Update $F((k-1)\delta) \mapsto F(k\delta)$
3. Re-minimize, i.e. is it now energetically favorable to move to a new state paying the frictional cost of moving the contact line,

$$\text{minimize } \ \mathcal{J}(w) + \operatorname{Diss}(u_\delta^{k-1}, w) \ \text{ over } w \in F(k\delta) + H_0^1(U).$$

4. repeat.

Minimizing movements limit

Using piecewise constant interpolation define, for all $t \in [0, T]$,

$$u_\delta(t) := u_\delta^k \ \text{ and } \ F_\delta(t) = F(k\delta) \ \text{ if } \ t \in [k\delta, (k+1)\delta).$$

The time incremental scheme converges *pointwise* in time in the limit $\delta \to 0$ via a compactness idea introduced by Mainik and Mielke ('05) (Helly's selection theorem).

We will call such pointwise limits *minimizing movements solutions*. Minimizing movements solutions are examples of *energy solutions*.

Energy solutions: PDE conditions

A measurable $u : [0, T] \to H^1(U)$ is a *energy solution* (E) if:

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Here $P(t) = P(u(t)) = \int_{\partial U} \frac{\partial u(t)}{\partial n}\, dS$ is an associated pressure.

PDE conditions: stability

Global minimization of

$$\mathcal{J}(u(t)) \leq \mathcal{J}(u') + \mathrm{Diss}(u(t), u') \qquad \text{for all } u' \in u(t) + H^1_0(U).$$

implies that $u(t)$ solves the local stability conditions

$$\begin{cases} \Delta u = 0 & \text{in } \{u > 0\} \cap U, \\ 1 - \mu_- \leq |\nabla u|^2 \leq 1 + \mu_+ & \text{on } \partial\{u > 0\} \cap U. \end{cases}$$

This is a typical first variation computation. So we are strengthening local stability to global stability.

Energy solutions: PDE conditions

A measurable $u : [0, T] \to H^1(U)$ is a *energy solution* (E) if:

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Here $P(t) = P(u(t)) = \int_{\partial U} \frac{\partial u(t)}{\partial n}\, dS$ is an associated pressure.

PDE conditions: dynamic slope

Computing the time derivative directly and integrating by parts

$$\frac{d}{dt}\mathcal{J}(u(t)) = \int_{\partial\Omega(t)} (1 - |\nabla u|^2) V_n \; dS + 2\dot{F}(t)P(t).$$

Differentiating energy dissipation balance

$$\frac{d}{dt}\mathcal{J}(u(t)) = 2\dot{F}(t)P(t) - \int_{\partial\Omega(t)} \mu_+(n)(V_n)_+ + \mu_-(n)(V_n)_- \; dS.$$

Combining the above two identities we find

$$\int_{\partial\Omega(t)} (1 + \mu_+ - |\nabla u|^2)(V_n)_+ + (|\nabla u|^2 - 1 + \mu_-)(V_n)_- \; dS = 0.$$

Both terms in the above integral are non-negative by stability, and so they must actually be zero pointwise.

Dynamic slope condition

Combining the above two identities we find

$$\int_{\partial\Omega(t)} (1 + \mu_+ - |\nabla u|^2)(V_n)_+ + (|\nabla u|^2 - 1 + \mu_-)(V_n)_- \; dS = 0.$$

implying that u solves, almost everywhere on $\partial\Omega(t)$,

$$\text{if } V_n > 0 \text{ then } |\nabla u|^2 = 1 + \mu_+$$

and

$$\text{if } V_n < 0 \text{ then } |\nabla u|^2 = 1 - \mu_-.$$

Here V_n is the outward normal velocity of $\Omega(t)$.

Local solution property

(Smooth) energy solutions $u(t)$ on $[0, T]$ satisfy the following local laws:

1. (*Local stability condition*) For all $t \in [0, T]$ the function $u(t) \in C(\overline{U})$ solves

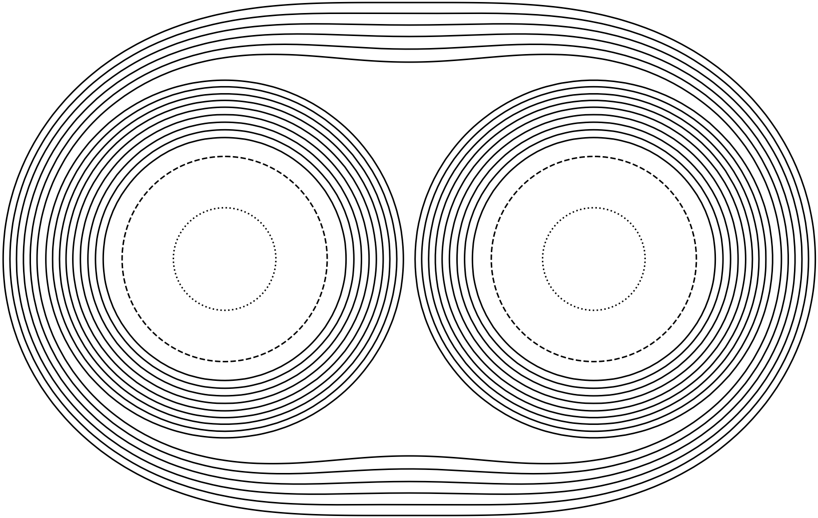
   $$\Delta u(t) = 0 \text{ in } \Omega(t) \text{ and } 1-\mu_- \leq |\nabla u(t)|^2 \leq 1+\mu_+ \text{ on } \partial\Omega(t).$$

2. (*Dynamic slope condition*) u solves

   $$|\nabla u|^2 = 1 \pm \mu_\pm \quad \text{if} \quad \pm V_n > 0 \quad \text{on } \partial\Omega(t) \cap U.$$

   Here V_n is the outward normal velocity of $\Omega(t)$.

Jumps occur “as early as possible”



Properties of general energy solutions

Theorem (F., Kim, Požár, preprint on arXiv)

Suppose u is an energy solution on $[0, T]$. Then

1. *(Basic regularity properties) The states $u(t)$ are uniformly Lipschitz and non-degenerate and $\mathcal{H}^{d-1}(\partial\Omega(t))$ is uniformly bounded in time. Also $t \mapsto \Omega(t)$ is in $BV([0, T]; L^1)$ and $u(t)$ has left and right limits in uniform metric at every time, denoted $u_\ell(t)$ and $u_r(t)$.*

2. *(Envelopes) The USC/LSC envelopes of u, called u^* and u_*, themselves solve* (E).

3. *(Dynamic slope condition a.e.) For all $t \in [0, T]$ the function $u(t)$ satisfies the stability condition (2) and satisfies (in terms of u^* and u_*) the dynamic slope condition (2) at $\mathcal{H}^{d-1}$ almost every point of its free boundary $\partial\Omega(t) \cap U$.*

Obstacle solutions

Local stability conditions

$$\begin{cases} \Delta u = 0 & \text{in } \{u > 0\} \cap U, \\ 1 - \mu_- \leq |\nabla u|^2 \leq 1 + \mu_+ & \text{on } \partial\{u > 0\} \cap U. \end{cases} \tag{2}$$

Assume F changes monotonicity at most on a finite set $Z \subset [0, T]$.

Definition

We say that $u : [0, T] \times \overline{U} \to [0, \infty)$ is an *obstacle solution* (O) if

1. (*Dirichlet forcing*) For all $t \in [0, T]$

$$u(t) = F(t) \text{ on } \partial U. \tag{3}$$

2. (*Initial data*) $u(0)$ is a solution of (2).
3. (*Obstacle condition*) For every $(s, t) \cap Z = \emptyset$, so that F is monotone on $[s, t]$, $u(t)$ is the minimal supersolution of (2) and (3) above $u(s)$ when F is increasing on $[s, t]$ (resp. maximal subsolution below $u(s)$ when F is decreasing).

Local solution property

Obstacle solutions $u(t)$ on $[0, T]$ satisfy the same local laws as energy solutions:

1. (*Local stability condition*) For all $t \in [0, T]$ the function $u(t) \in C(\overline{U})$ is a continuous viscosity solution of

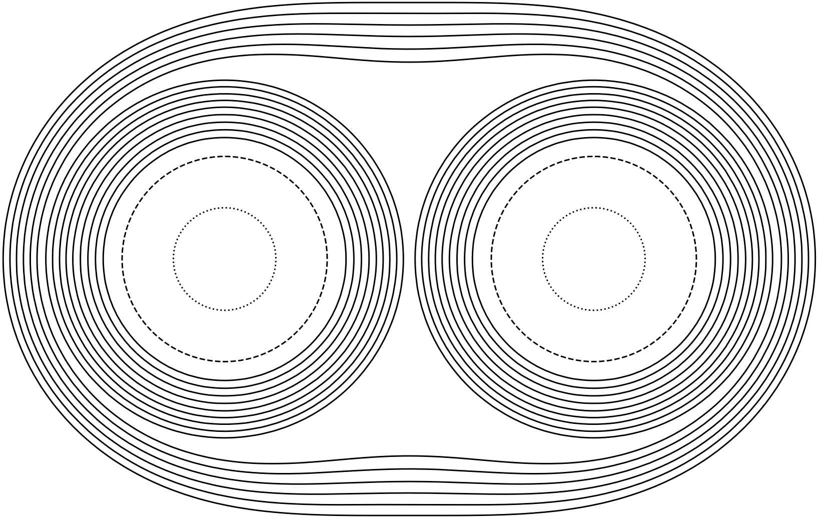
   $$\Delta u(t) = 0 \text{ in } \Omega(t) \text{ and } 1 - \mu_- \leq |\nabla u(t)|^2 \leq 1 + \mu_+ \text{ on } \partial\Omega(t).$$

2. (*Dynamic slope condition*) u is a (semicontinuous envelope) viscosity solution on $[0, T] \times U$ of

   $$|\nabla u|^2 = 1 \pm \mu_\pm \quad \text{if} \quad \pm V_n > 0 \quad \text{on } \partial\Omega(t) \cap U.$$

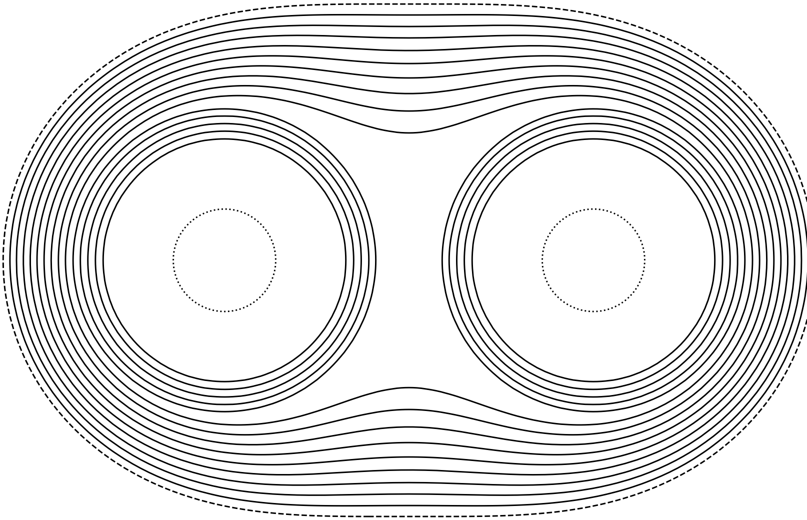
   Here V_n is the outward normal velocity of $\Omega(t)$.

Simulation: two annuli scenario

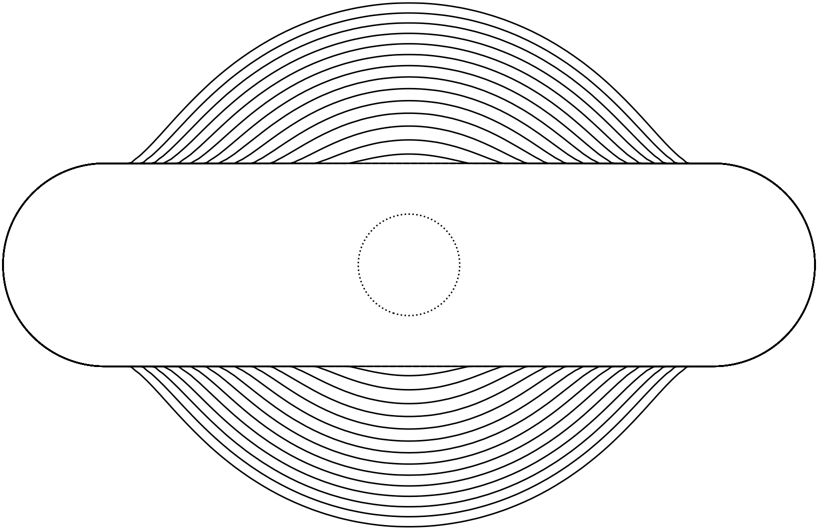


Scheme based on [Gibou et al ‘02], simulations by N. Požár

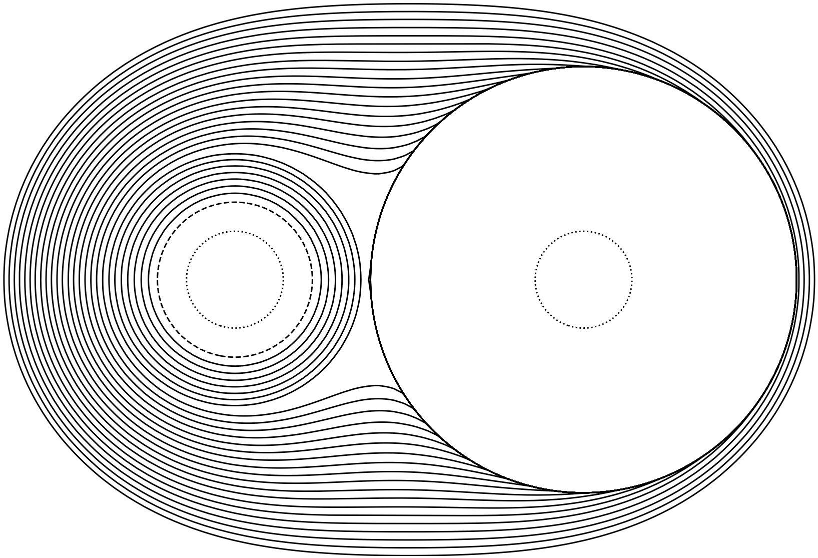
Simulation: two annuli reversed



Simulation: de-pinning geometry



Simulation: two different annuli



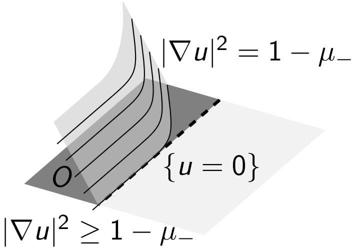
Star-shaped geometry

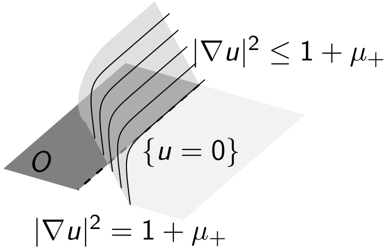
Theorem (F., Kim, Požár, preprint on arXiv)

Suppose that $\mathbb{R}^d \setminus U$ and Ω_0 are strongly star-shaped and bounded, Ω_0 is C^2, and $F : [0, T] \to (0, \infty)$ is Lipschitz and only changes monotonicity finitely many times. Let u be the unique obstacle solution on $[0, T]$. Then

1. *The profile $u(t)$ is strongly star-shaped for each time. The positivity set $\Omega(t)$ and the profile $u(t)|_{\Omega(t)}$ have the regularity $L^\infty_t C_x^{1,\frac{1}{2}-}$.*
2. *If $v(t)$ is another profile with the same forcing $F(t)$ and also satisfies the local stability and dynamic slope condition in the weak (comparison) sense then $v \equiv u$.*
3. *The solutions of the discrete-time minimizing scheme converge uniformly to $u(t)$ with a uniform rate that only depends on F, $\mu_\pm$ and d.*

Origin of the regularity: one-phase obstacle problems





Expansion of ε-flat solutions near the de-pinning boundary

$$u(x) = (1 \pm \mu_\pm)^{1/2}(x_n \pm \varepsilon w(x) + o(\varepsilon))_+ \quad \text{in} \quad B_1$$

where w solves the Signorini / thin obstacle problem:

$$\Delta w = 0 \quad \text{in} \quad B_1^+, \ \min\{-\partial_{x_n} w, w\} = 0 \quad \text{on} \quad B_1'.$$

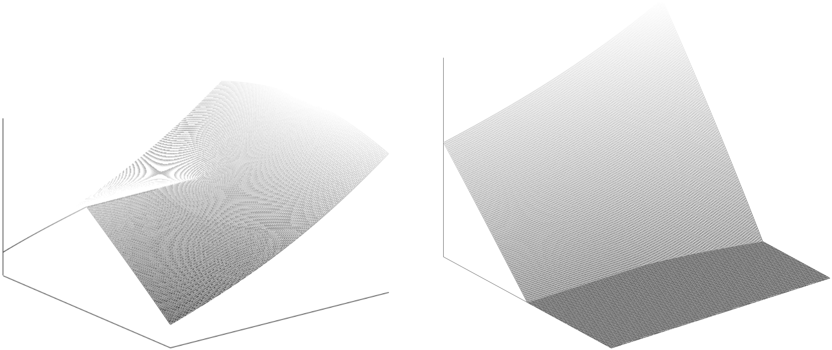
[Chang-Lara and Savin] and [Ferreri and Velichkov]

Signorini optimal regularity

Signorini problem optimal regularity is $C^{1,\frac{1}{2}}$ due to the special solution

$$w(x_1, x_2) = \mathrm{Re}((x_1 + ix_2)^{3/2})$$

which corresponds to an approximate solution of the Bernoulli obstacle problem $u(x) = (1 \pm \mu_\pm)^{1/2}(x_2 + \varepsilon w)_+$.



Minimizing movements solutions in general geometry

In general geometry jumps occur and are a serious challenge.
Recall that *minimizing movements solutions* are pointwise in time limits of the scheme

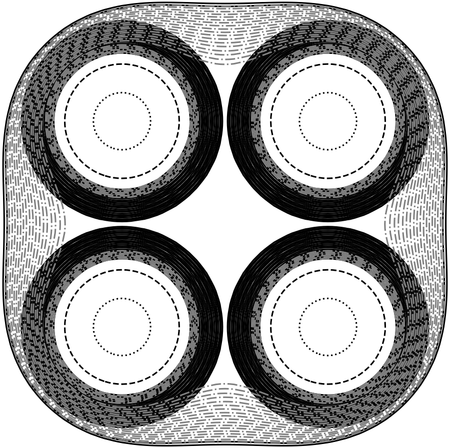
$$u_\delta(t_k) \in \mathcal{M}[u_\delta(t_{k-1}), F(t_k)],$$

where

$$\mathcal{M}[u, F] := \operatorname{argmin}\{\mathcal{J}(w) + \mathsf{Diss}(u, w) : w \in H^1_0(U) + F\} \quad (4)$$

and $t_k \in \mathcal{P}_\delta$ are in some sequence of δ-width partitions $\mathcal{P}_\delta$.

Jumps at a monotonicity change cause branching non-uniqueness



Description of minimizing movements solutions: monotone case

Theorem (Collins and F., forthcoming)

Suppose that $F(t, x)$ is strictly monotone in t on $[0, T]$. To avoid initial data that jumps immediately, we assume stability: $u(0) \in \mathcal{M}[u(0), F(0)]$. Then $\mathcal{M}[u(0), F(t)]$ is a singleton except for countably many times, and all minimizing movements solutions $u(t)$ satisfy

$$u(t) \in \mathcal{M}[u(0), F(t)] \quad \textit{for} \quad t \in [0, T].$$

In other words, like in the case of obstacle solutions, the minimizing movements scheme for monotone forcing is just an (energetic analogue) of the Bernoulli obstacle problem with a single obstacle and a continuous family of boundary data.

Description of minimizing movements solutions: piecewise monotone case

Theorem (Collins and F., forthcoming)

Let $0 = t_0 < \cdots < t_N = T$ *and suppose that* $F(t, x)$ *is strictly monotone in* t *on each* $[t_j, t_{j+1}]$. *To avoid initial data that jumps immediately, we assume stability:* $u(t_0) \in \mathcal{M}[u(t_0), F(t_0)]$.
Then any sequence $u(t_i)$, *chosen recursively by*

$$u(t_i) \in \mathcal{M}[u(t_{i-1}), F(t_i)],$$

defines a minimizing movements solution at the intervening times via

$$u(t) \in \mathcal{M}[u(t_i), F(t)] \qquad t \in (t_i, t_{i-1})$$

This is a genuine definition of u, *in the sense that all solutions with the same* $u(t_i)$ *jump at the same times and agree up to value at jumps. Conversely, all minimizing movements solutions have the form (6).*

Regularity of minimizing movements solutions

This uniqueness property reduces the evolution to a finite family of Bernoulli obstacle problems with recursively defined obstacles. We can then apply the regularity theory of Bernoulli obstacle problems from Chang-Lara and Savin, and Ferreri and Velichkov to derive.

Theorem (Collins and F., forthcoming)

Suppose that $d = 2$ and $F : [0, T] \to C^\infty(\partial U)$ is piecewise monotone in t, and u is a **minimizing movements solution** *on $[0, T]$. Then $u \in L^\infty_t C^{1,\frac{1}{2}-}$.*

In higher dimensions Bernoulli minimizers may have singularities so the statement is more complicated.

Future directions

- Uniqueness of energy solutions in star-shaped case? Does the dynamic slope condition hold everywhere instead of almost everywhere?
- Connection between obstacle solutions and *balanced viscosity solutions*.
- Volume constraint case.
- Derivation by stochastic homogenization.
- Is there an energetic formulation in the case of anisotropic pinning interval? Such problems naturally arise from periodic homogenization, but the induced dissipation rate functional does not seem to be associated with any “good” global dissipation distance.

Thanks for your attention!