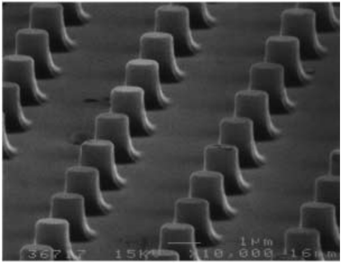
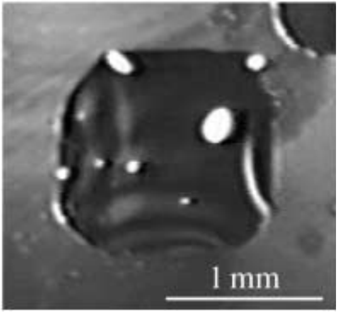
Interfaces in inhomogeneous media: pinning, hysteresis, and facets

Will Feldman

The University of Utah

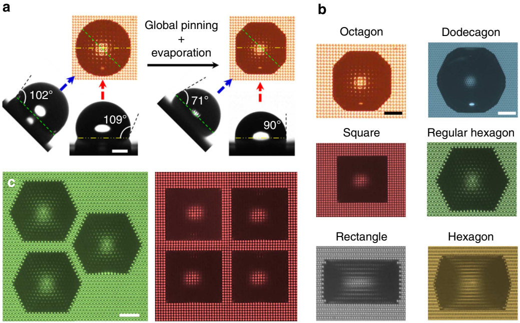
Liquid drops on rough surfaces





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

Liquid drops on rough surfaces



Raj, Adera, Enright and Wang *Nat. Commun.* (2014)

Capillarity model

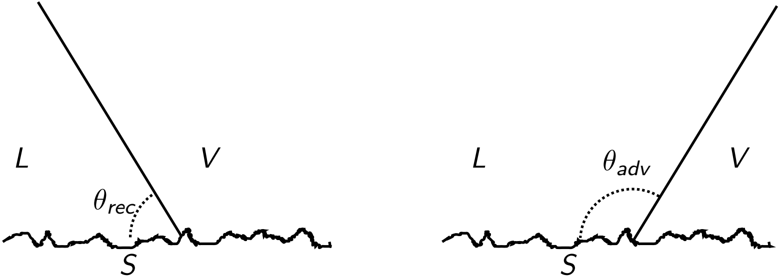
Energy of liquid (L), vapor (V) and solid (S) configuration

$$E = \sigma_{\mathsf{LV}}|\partial L \cap \partial V| + \sigma_{\mathsf{SL}}|\partial S \cap \partial L| + \sigma_{\mathsf{SV}}|\partial S \cap \partial V|$$

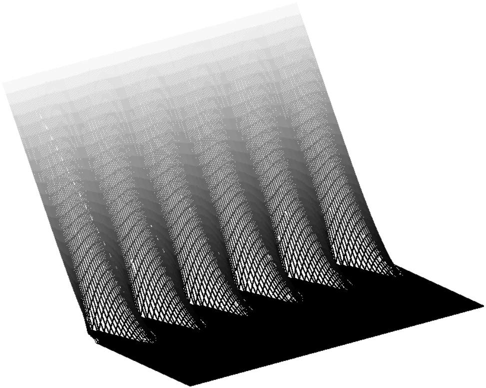
Energy minimizers satisfy contact angle condition,

$$\cos\theta_Y = (\sigma_{\mathsf{SV}} - \sigma_{\mathsf{SL}})/\sigma_{\mathsf{LV}}.$$

Rough surface has **contact angle hysteresis**, range of stable effective contact angles (**pinning interval**):



Pinned angle visualization



A simpler model

Alt-Caffarelli energy functional of a height profile $u : \mathbb{R}^d \to [0, \infty)$:

$$J[u] = \int_U Q(\tfrac{x}{\varepsilon})^2 \, 1_{\{u>0\}}(x) + |\nabla u(x)|^2 \, dx$$

Q is $\mathbb{Z}^d$-periodic and positive.

Associated Euler-Lagrange equation:

$$\begin{cases} \Delta u^\varepsilon = 0 & \text{in } \{u^\varepsilon > 0\} \text{ and} \\ |\nabla u^\varepsilon| = Q(\tfrac{x}{\varepsilon}) & \text{on } \partial\{u^\varepsilon > 0\}. \end{cases}$$

Interval of pinned slopes

For $p \in \mathbb{R}^d \setminus \{0\}$ and look for solution $v : \mathbb{R}^d \to [0, \infty)$ to

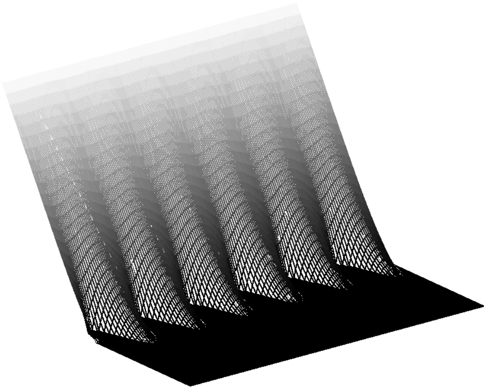
$$\begin{cases} \Delta v(x) = 0 \quad \text{in } \{v > 0\} \\ |\nabla v(x)| = Q(x) \quad \text{on } \partial\{v > 0\} \\ \sup_{\mathbb{R}^d} |v(x) - (p \cdot x)_+| < \infty. \end{cases}$$

These are called plane-like solutions. Call a slope pinned if there exists a plane-like solution with slope p. Define for $e \in S^{d-1}$

$$Q_*(e) = \inf\{\alpha : \ \alpha e \text{ is pinned}\} \ \text{ and } \ Q^*(e) = \sup\{\alpha : \ \alpha e \text{ is pinned}\}.$$

(Caffarelli and de la Llave, Caffarelli and Lee)

Pinned slope visualization



Limit shapes

Complicated multiscale problem

$$\Delta u^\varepsilon = 0 \text{ in } \{u^\varepsilon > 0\} \text{ and } |\nabla u^\varepsilon| = Q(\tfrac{x}{\varepsilon}) \text{ on } \partial\{u^\varepsilon > 0\}.$$

Effective problem describes large scale shapes as $\varepsilon \to 0$

$$\Delta \bar{u} = 0 \text{ in } \{\bar{u} > 0\} \text{ and } |\nabla \bar{u}| \in [Q_*(n_x), Q^*(n_x)] \text{ on } \partial\{\bar{u} > 0\}.$$

Recovery sequence: given a solution u to the effective problem is there a sequence u^ε solving the ε-problem and $u^\varepsilon \to u$.

Theorem (F., ARMA '21)

Results in $d = 2$:

- *Existence of recovery sequences (convex data).*
  - *Effective problem solutions correspond to large scale shapes of rough surface solutions.*
- *Continuity/discontinuity of pinning interval + examples.*
  - *Formation of facets at the limit problem.*

An "even simpler" model

Discrete Alt-Caffarelli functional, for $u : \mathbb{Z}^d \to [0, \infty)$ and $\Lambda \subset \mathbb{Z}^d$ define:

$$J[u] = \sum_{\Lambda} 1_{\{u>0\}}(x) + d \sum_{|x-y|=1,\ \{x,y\}\cap\Lambda\neq\emptyset} (u(y) - u(x))^2.$$

Euler-Lagrange equation with respect to single site variations:

$$\begin{cases} \Delta_{\mathbb{Z}^d} u = 0 & \text{in } \{u > 0\} \\ \Delta_{\mathbb{Z}^d} u \leq 1 & \text{on } \partial_{out}\{u > 0\}, \\ u \geq \frac{1}{2d} & \text{on } \partial_{in}\{u > 0\}. \end{cases}$$

Effective problem describes large scale shapes

$$\begin{cases} \Delta \bar{u} = 0 & \text{in } \{\bar{u} > 0\} \\ |\nabla \bar{u}| \in [H_*(n_x), H^*(n_x)] & \text{on } \partial\{\bar{u} > 0\} \end{cases}$$

Discrete model: minimal supersolutions

An associated evolution

Let $N \in \mathbb{N}$ large and $u(x,0) = N\,1_{B_N(0)}(x)$.

Define an evolution, for $t \in \mathbb{N}$ and $x \in \mathbb{Z}^d \setminus B_N$,

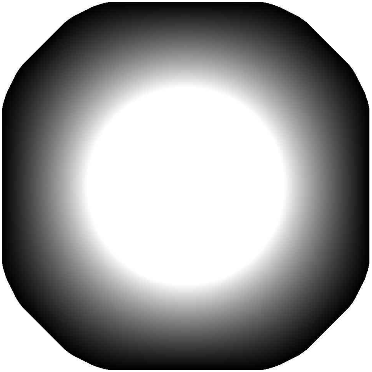
$$u(x,t+1) = u(x,t) + (2d)^{-1} \max\{0, \Delta_{\mathbb{Z}^d} u(x,t) - 1_{\{u_t=0\}}(x)\}.$$

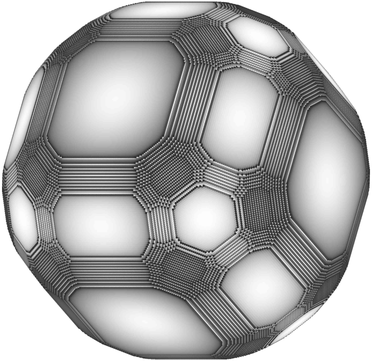
It is not hard to check that this stabilizes in the limit $t \to \infty$ to the minimal supersolution of

$$\begin{cases} \Delta_{\mathbb{Z}^d} u_N = 0 & \text{in } \{u_N > 0\} \setminus B_N, \\ \Delta_{\mathbb{Z}^d} u_N \le 1 & \text{on } \partial_{out}\{u_N > 0\} \setminus B_N, \end{cases} \quad \text{with} \quad u_N = N \ \text{ on } B_N.$$

This is basically the boundary sandpile model introduced by Aleksanyan and Shahgholian.

Scaling limit?





Scaling limit?

Consider the minimal solutions of

$$\begin{cases} \Delta_{\mathbb{Z}^d} u_N = 0 & \text{in } \{u_N > 0\} \setminus B_N, \\ \Delta_{\mathbb{Z}^d} u_N \leq 1 & \text{on } \partial_{out}\{u_N > 0\} \setminus B_N, \end{cases} \quad \text{with} \quad u_N = N \quad \text{on } B_N.$$

Lipschitz estimate, standard in free boundary regularity theory, tells us that the rescalings

$$\bar{u}_N(x) = N^{-1} u_N(Nx)$$

are uniformly bounded and equicontinuous.

We need to show that the limit

$$\bar{u} = \lim_{N \to \infty} \bar{u}_N$$

solves a PDE.

Effective free boundary condition

For $e \in S^{d-1}$ define $H^*(e)$ to be the largest α such that there exists a global supersolution

$$\Delta_{\mathbb{Z}^d} v \leq 0 \ \text{ in } \ \{v > 0\}, \ \Delta_{\mathbb{Z}^d} v \leq 1 \ \text{ on } \ \partial_{out}\{v > 0\}$$

and

$$v(0) = 0 \ \text{ with } \ v(x) \geq \alpha(e \cdot x)_+.$$

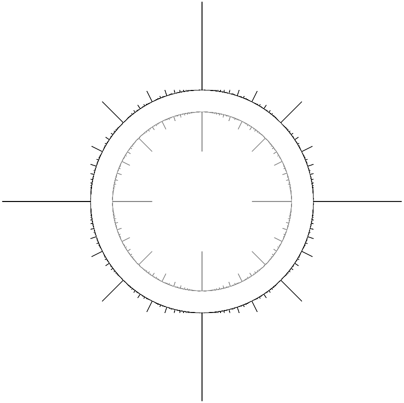
Theorem (Smart and F., ARMA '18)

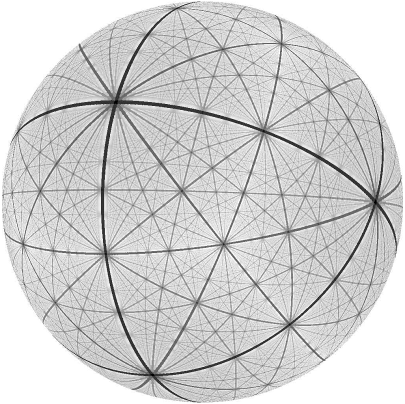
The $\bar{u}_N$ converge uniformly on $\mathbb{R}^d$ to $\bar{u}$ which is the unique viscosity solution (and minimal supersolution) of

$$\begin{cases} \Delta \bar{u} = 0 & \text{in } \{\bar{u} > 0\} \setminus B_1, \\ |\nabla \bar{u}| = H^*(n_x) & \text{on } \partial\{\bar{u} > 0\} \setminus B_1, \end{cases} \quad \text{with } \ \bar{u} = 1 \text{ on } B_1.$$

Furthermore $\{\bar{u} > 0\}$ is convex and has a nontrivial facet at every rational direction.

Structure of the effective PDE





Structure of the effective PDE

Theorem (Smart and F., ARMA '18)

Define $S : 2\pi\mathbb{T}^d \to \mathbb{R}$ *by* $S(\theta) = -\log(1 + \frac{1}{d}\sum_{j=1}^d \cos\theta_j)$*, and let* $\hat{S} : \mathbb{Z}^d \to \mathbb{C}$ *be the corresponding Fourier transform. Then* $\hat{S}$ *is real and positive on* $\mathbb{Z}^d$ *and for all* $e \in S^{d-1}$*,*

$$H^*(e) = \frac{1}{\sqrt{2d}} \exp\left(\frac{1}{2} \sum_{k \in \mathbb{Z}^d:\ k \cdot e = 0} \hat{S}(k) \right).$$

Minimal supersolution

Need to show existence of a sequence of (rescaled) discrete supersolutions $\tilde{u}_N$ converging to $\bar{u}$. Theory of viscosity solutions allows us to localize and only argue for smooth test functions.

New theory needs to be developed due to the discontinuous free boundary condition.

Theorem (Smart and F., ARMA '18)

Strict comparison principle holds for

$$\Delta u = 0 \;\; \textit{in} \;\; \{u > 0\} \;\; \textit{with} \;\; H^*(\nabla u) = 1 \;\; \textit{on} \;\; \partial\{u > 0\}$$

when $d = 2$ or in arbitrary dimension and convex setting.

Continuous model

Outline

Recall the continuous model

$$\begin{cases} \Delta u^\varepsilon = 0 & \text{in } \{u^\varepsilon > 0\} \\ |\nabla u^\varepsilon| = Q(\frac{x}{\varepsilon}) & \text{on } \partial\{u^\varepsilon > 0\}. \end{cases}$$

- Step 1: Identify the minimal and maximal effective slopes
  - Plane-like solutions (Caffarelli-de la Llave, Caffarelli-Lee, Kim)
- Step 2: Convergence of minimal and maximal solutions
  - Comparison principle for limit problem (Smart and F.)
  - Foliations/laminations by plane-like solutions (F.)
- Step 3: Recovery sequences for general solutions (F.)

Effective slopes

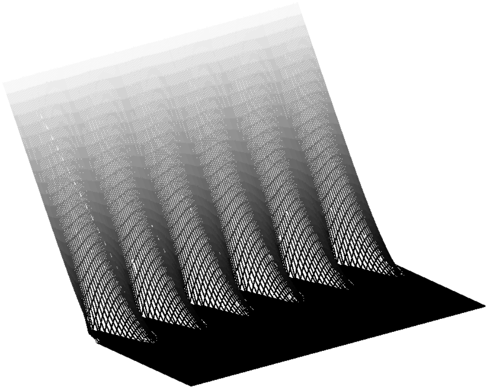
For $p \in \mathbb{R}^d \setminus \{0\}$ and look for solution $v : \mathbb{R}^d \to [0, \infty)$ to

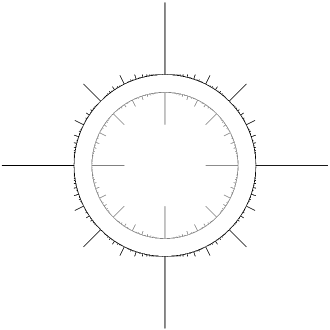
$$\begin{cases} \Delta v(x) = 0 \quad \text{in } \{v > 0\} \\ |\nabla v(x)| = Q(x) \quad \text{on } \partial\{v > 0\} \\ \sup_{\mathbb{R}^d} |v(x) - (p \cdot x)_+| < \infty. \end{cases}$$

These are called plane-like solutions. Call a slope pinned if there exists a plane-like solution with slope p. Define for $e \in S^{d-1}$

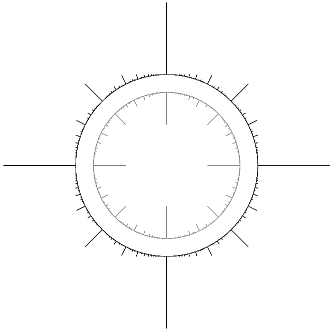
$$Q_*(e) = \inf\{\alpha : \ \alpha e \text{ is pinned}\} \ \text{ and } \ Q^*(e) = \sup\{\alpha : \ \alpha e \text{ is pinned}\}.$$

Recovery sequence: geometric viewpoint

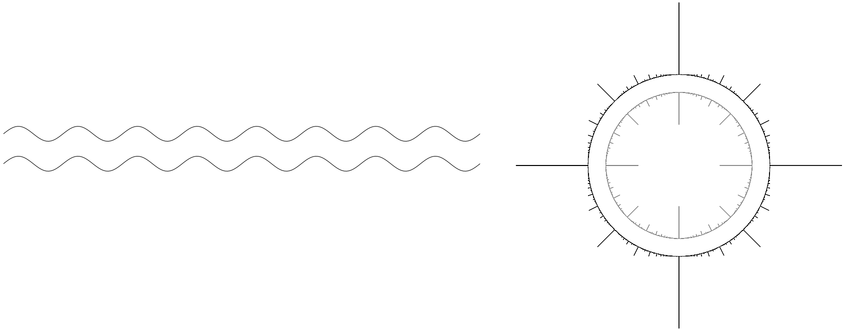




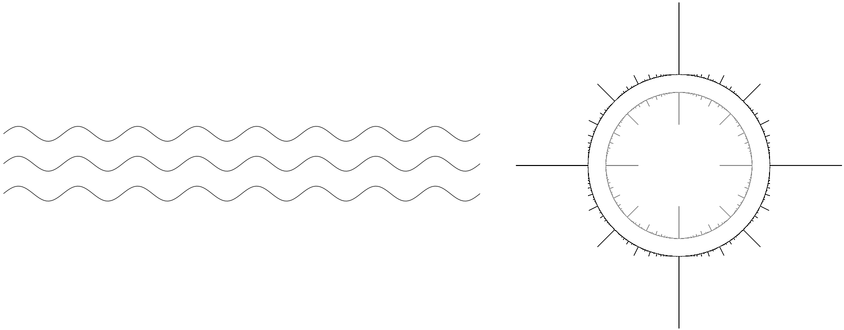
Recovery sequence: geometric viewpoint



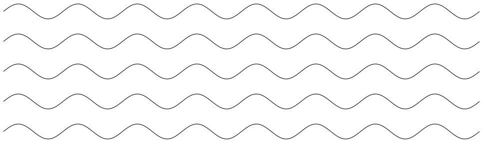
Recovery sequence: geometric viewpoint

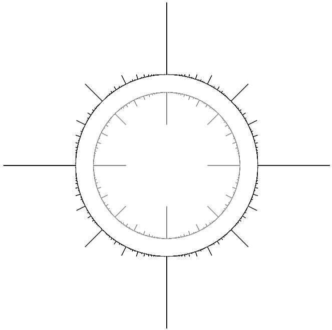


Recovery sequence: geometric viewpoint

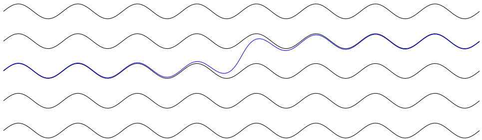


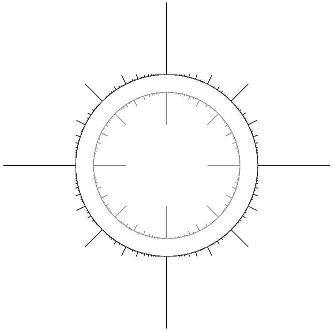
Recovery sequence: geometric viewpoint



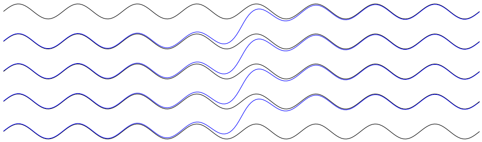


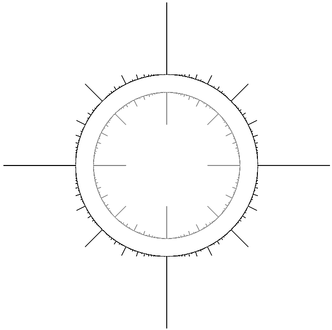
Recovery sequence: geometric viewpoint



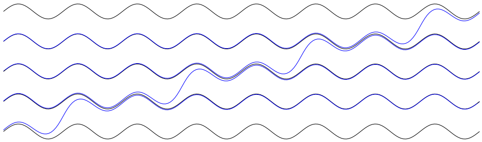


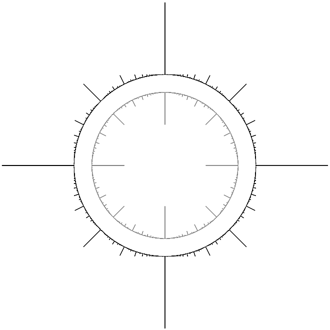
Recovery sequence: geometric viewpoint





Recovery sequence: geometric viewpoint



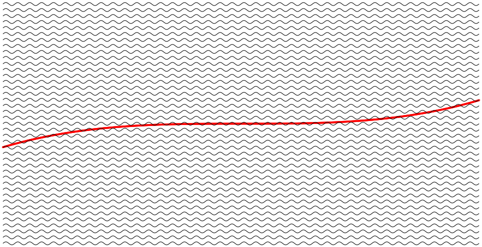


Recovery sequence: geometric viewpoint

$\partial\{\bar{u} > 0\}$

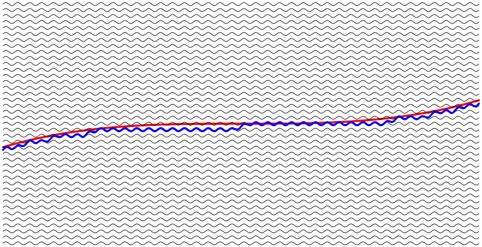
Recovery sequence: geometric viewpoint

$\partial\{\bar{u} > 0\}$



Recovery sequence: geometric viewpoint

$\partial\{\bar{u} > 0\}$



The takeaway

Free boundary problem with rough surface

$$\Delta u^\varepsilon = 0 \text{ in } \{u^\varepsilon > 0\} \quad \text{and} \quad |\nabla u^\varepsilon| = Q(\tfrac{x}{\varepsilon}) \text{ on } \partial\{u^\varepsilon > 0\}.$$

Effective *pinning problem*

$$\Delta \bar{u} = 0 \text{ in } \{\bar{u} > 0\} \quad \text{and} \quad |\nabla \bar{u}| \in [Q_*(n_x), Q^*(n_x)] \text{ on } \partial\{\bar{u} > 0\}.$$

- The pinning problem describes large scale shapes of rough surface solutions as $\varepsilon \to 0$.
- Qualitative properties (e.g. facets) of effective free boundary depends on continuity properties of the pinning interval.
- Pinning interval properties can be studied via the plane-like solutions.
- Minimal and maximal solutions play a very important role.

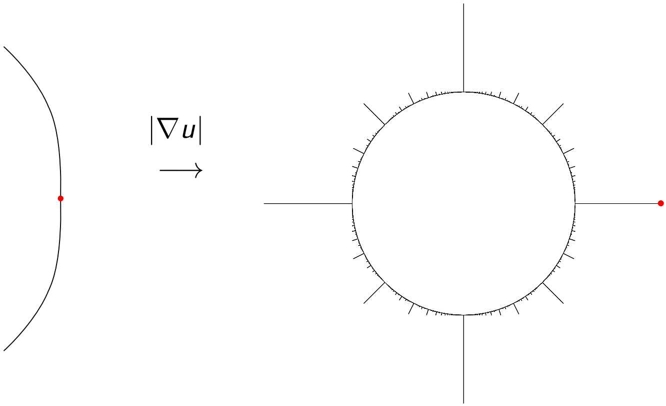
Future Directions / Open Questions

- Optimal regularity of the free boundary for the discontinuous free boundary condition. We know at least C^1 from convexity + blow up argument.
- Presence of facets with co-dimension ≥ 2.
- General comparison principle and explaining facet shapes in $d \geq 3$.
- Shapes of local minimizers for the discrete model.
- Energy based approach, perhaps via dissipative evolutions, volume constrained solutions.
- Random media.
- What phenomena need to be explained with rough surface (as opposed to chemically patterned)?

Thank you for your attention!

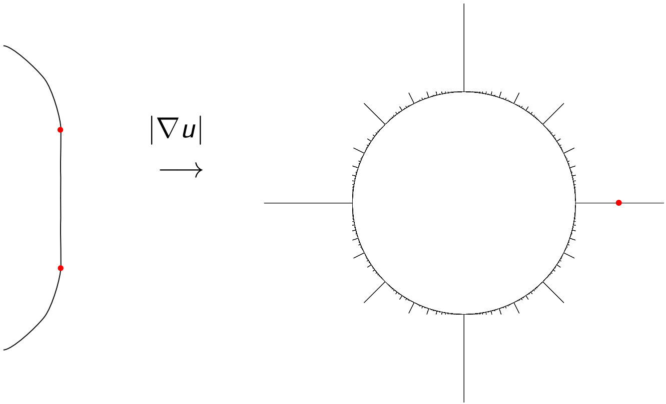
Discontinuities in H^* cause facets

Idea of Caffarelli and Lee:



Discontinuities in H^* cause facets

Idea of Caffarelli and Lee:



Discontinuities in H^* cause facets

Idea of Caffarelli and Lee: