Sharp isoperimetric inequality, discrete PDEs and Semidiscrete optimal transport

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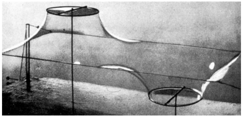
March 2, 2021

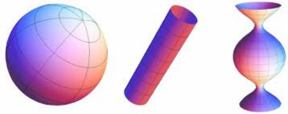
Geometric motivations

Σ_t surface, then $\frac{d}{dt}\Big|_{t=0} \text{Area}(\Sigma_t) = 0$: Minimal Surfaces $CM = 0$.



Otto Frei, 1964

$\frac{d}{dt}\Big|_{\substack{t=0\\ |\Omega_t|=1}} \text{Area}(\partial\Omega_t) = 0$: Constant mean curvature $CM = \lambda$.

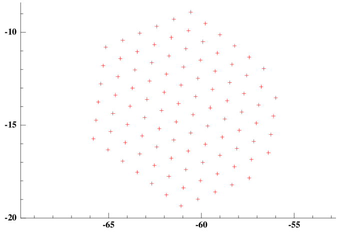


Classical problem: $\min\left\{\text{Area}(\partial\Omega) : |\Omega| = 1\right\}$. Solution: $\Omega = B$.

How to translate these classical principles to the discrete world?

Physical motivations

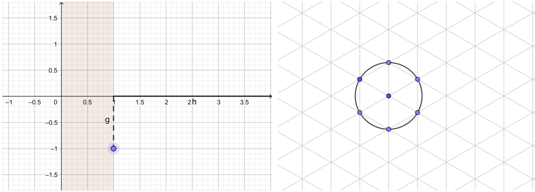
Minimize $\sum_{i\neq j} V(|x_i - x_j|)$ with $V(r) = \frac{1}{r^{12}} - \frac{1}{r^6}$ or similar:



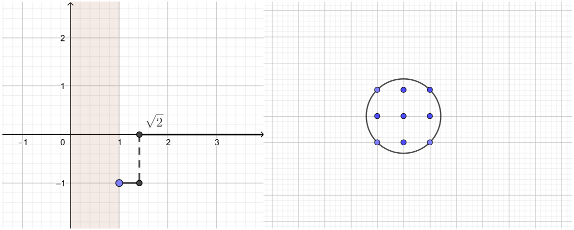
Survey by Blanc-Lewin 2015, $N = 100$

Tóth 1956, Heitmann-Radin 1980: sticky disk rigidity.
Schmidt 2013, De Luca-Friesecke 2017: $N^{3/4}$-fluctuations around hexagon (sticky disc).
Theil 2006: minimizer resistent to perturbations of V (in the limit $N \to \infty$)
Bétermin-Petrache 2018 observation: $\mathbb{Z}^2$ sometimes outperforms A_2.
Bétermin-De Luca-Petrache 2018: crystallization to $\mathbb{Z}^2$ for "sticky shell" model (robust under perturbation).

SIMPLIFIED MODELS



Tóth, Heitmann-Radin "Sticky discs"



Bétermin-De Luca-Petrache "Sticky shells"?

What's the crystal shape?

(Discrete isoperimetric problems)

CONTINUUM ISOPERIMETRIC INEQUALITIES

Find $H \subset \mathbb{R}^d$ such that for all $\Omega \subset \mathbb{R}^d$: $\quad \dfrac{\mathrm{Area}(\partial H)^d}{\mathrm{Vol}(H)^{d-1}} \leq \dfrac{\mathrm{Area}(\partial\Omega)^d}{\mathrm{Vol}(\Omega)^{d-1}}$

- Equivalently: H minimizes perimeter at fixed volume.
- Can be extended to general notions of "$\mathrm{Vol}(\Omega)$" and "$\mathrm{Area}(\partial\Omega)$":

$$\left.\begin{aligned} P_g(\Omega) &:= \int_{\partial\Omega} g(\nu(x))dS(x) \\ V_w(\Omega) &:= \int_\Omega w(x)dV(x) \end{aligned}\right\} \quad \text{con} \quad H : \mathbb{R}^d \to \mathbb{R} \begin{cases} w, g \geq 0, \\ H(\lambda x) = \lambda H(x) \\ H \text{ convex} . \end{cases}$$

- **In this talk we only consider $w = 1$ for simplicity.**
- Optimizer $H = \{x \in \mathbb{R}^d : \ \forall \nu, \ x \cdot \nu < g(\nu)\}$ **Wulff 1901**.
- **Del Nin - Petrache 2021**: discrete-continuum limit for crystals and quasicrystals.

Continuum case proofs – 1/4

Strategy 1: PDE + convexity

(**Cabré-Ros Oton-Serra 2013, Trudinger 1994**)

$$\begin{cases} \Delta u(x) = \frac{P_g(\Omega)}{|\Omega|} & x \in \Omega, \\ \frac{\partial u}{\partial \nu}(x) = g(\nu(x)) & x \in \partial\Omega. \end{cases}$$

Solution exists, is regular and unique up to constant summand.

$$\partial_\Omega u := \{x \in \Omega : \ u(y) \geq u(x) + \nabla u(x) \cdot (y - x) \quad y \in \overline{\Omega}\}.$$

(x such that tg. plane to graph of u at x supports graph$(u|_\Omega)$.)

Continuum case proofs – 2/4

Claim: $H \subset \nabla u(\partial_\Omega u)$.

- $p \in H$ means: $p \cdot \nu < g(\nu)$ for all $\nu \in \mathbb{S}^{d-1}$.
- Let $x \in \overline{\Omega}$ min of $u(y) - p \cdot y$.
- If $p \in \partial\Omega$ then $\frac{\partial(u(y)-p\cdot y)}{\partial \nu} \leq 0 \Leftrightarrow \frac{\partial u}{\partial \nu}(x) \leq p \cdot \nu < g(\nu)$, contradiction.
- So x is interior. It follows:
  - $p = \nabla u(x)$ (u smooth),
  - $u(y) \geq u(x) + p \cdot (y - x)$ (for all $y \in \overline{\Omega}$).

  Therefore $p \in \nabla u(\partial_\Omega u)$, proving the claim.

We get $$|H| \leq |\nabla u(\partial_\Omega u)| = \int_{\nabla u(\partial_\Omega u)} dp \leq \int_{\partial_\Omega u} \det[D^2 u(x)] dx$$

Continuum case proofs – 3/4

Linear algebra: $\lambda_1 \le \lambda_2 \le \cdots \le \lambda_d$ eigenvalues of $D^2u(x)$, then

$$\det[D^2u(x)] = \prod_{j=1}^{d} \lambda_j \le \left(\frac{1}{d} \sum_{j=1}^{d} \lambda_j \right)^d = \left(\frac{\mathrm{tr}[D^2u(x)]}{d} \right)^d = \left(\frac{\Delta u(x)}{d} \right)^d .$$

We get:

$$|H| \le |\partial_\Omega u| \left(\frac{\Delta u(x)}{d} \right)^d = |\partial_\Omega u| \left(\frac{P_g(\Omega)}{d \cdot |\Omega|} \right)^d \le |\Omega| \left(\frac{P_g(\Omega)}{d \cdot |\Omega|} \right)^d .$$

$$\frac{|H|}{d^d} \le \frac{P_g(\Omega)^d}{|\Omega|^{d-1}} .$$

Finally, due to the duality $W \leftrightarrow H$:

$$P_g(H) = \int_{\partial H} g(\nu(x)) dS \overset{*}{=} \int_{\partial H} x \cdot \nu(x) dS = \int_H \mathrm{div}(x) dx = d|H| .$$

Continuum case proofs – 4/4

Strategy 2: Mass transportation proof (sketch)

(Cordero Erausquin - Nazaret - Villani 2004, Figalli-Maggi-Pratelli 2010, Gromov 1983)

- Let $T : \Omega \to H$ transport density $\frac{|H|}{|\Omega|} 1_\Omega(x)$ to $1_H(x)$.
- $g^*(y) := \min\{\lambda > 0 : \ \lambda y \in H\}$ dual norm to g.
- Then $g^*(T(x)) \leq 1$ for a.e. $x \in \Omega$.

$$\begin{aligned}
d|\Omega| \left(\frac{|H|}{|\Omega|}\right)^{\frac{1}{d}} &= d \int_\Omega (\det \nabla T)^{\frac{1}{d}} dx \\
&\leq \int_\Omega \operatorname{div} T \, dx = \int_{\partial^* \Omega} T \cdot \nu_\Omega \, dS \\
&\leq \int_{\partial^* \Omega} g^*(T(x)) g(\nu_\Omega(x)) dS \leq P_g(\Omega).
\end{aligned}$$

Discrete sharp isoperimetric inequality

Setup:

- $V \subset \mathbb{R}^d$ possible positions of points (atoms).
- $G = (V, E)$ undirected graph of possible edges (bonds).
- $g : E \to [0, +\infty)$ weight (energy) of edges.

Looking for edge-isoperimetric inequalities of the form

$$\forall \Omega \subset V \text{ finite}, \quad (\sharp\Omega)^{d-1} \le C(\sharp_g \partial\Omega)^d := C \left(\sum_{(x,y) \in \overrightarrow{\partial\Omega}} g(x, y) \right)^d .$$

- Sharp inequality: Equality actually achieved for some $\Omega \subset V$.
- Interesting case: Equality achieved for ∞-many values of $\sharp\Omega$.

Sample results

- **Hamamuki 2014**: $\mathbb{Z}^d$ product graph with nearest-neighbor edges, constant g (cubes optimize).
- **Gomez-Petrache 2020**: The triangular lattice (with $g = 1$) does not have a sharp inequality as above, but rather

$$\frac{(\sharp\overrightarrow{\partial\Omega} - 6)^2}{4\sharp\Omega - \sharp\overrightarrow{\partial\Omega} + 2} \geq 12,$$

  optimized only by "perfect hexagons" (follows via result for honeycomb graph).
- **Gomez-Petrache 2020**: In honeycomb graph hexagons optimize.
- **Gomez-Petrache 2020**: In the 1-skeleton of the Voronoi diagram of the BCC, rhombic dodecahedron configurations optimize.
- **Gomez-Petrache 2020**: Sharp inequalities occur for special geometries of V, such as reciprocals of Coxeter triangulations.

The discrete result

- Auxiliary symmetric $A : V \times V \to \mathbb{R}$ with $E = \{A = 0\}$, defines Laplacian $\Delta_A u(x) := \sum_{y \in V} A^2(y,x)(u(x) - u(y))$.
- Solve discrete PDI (discrete PDE not solvable in general)

$$\begin{cases} \Delta_A u(x) \le \frac{1}{\sharp\Omega} \sum_{(x,y)\in\overrightarrow{\partial\Omega}} g(x,y) & \text{for } x \in \Omega \\ u(y) - u(x) = \frac{g(x,y)}{A(x,y)} & \text{for } (x,y) \in \overrightarrow{\partial\Omega}. \end{cases}$$

- Some notations:

$$\begin{aligned} \partial u(x) &:= \{p \in \mathbb{R}^d : \ (\forall z \in \overline{\Omega}),\ u(x) \le u(z) + p\cdot(x-z)\}, \\ \partial^{\mathrm{prox}} u(x) &:= \{p \in \mathbb{R}^d : \ (\forall z : \ z \sim x),\ u(x) \le u(z) + p\cdot(x-z)\}, \\ H_g &:= \left\{p \in \mathbb{R}^d : \ (\forall (x,y) \in \overrightarrow{\partial\Omega}),\ p\cdot(y-x) \le \frac{g(x,y)}{A(x,y)}\right\}. \end{aligned}$$

The discrete result (Gomez-Petrache 2020)

We find an analogue to strategy 1:

$$
\begin{aligned}
|H_g| &\overset{(a)}{\leq} \left| \bigcup_{x\in\Omega} \partial u(x) \right| \overset{(b)}{=} \sum_{x\in\Omega} |\partial u(x)| \\
&\overset{(c)}{\leq} \sum_{x\in\Omega} |\partial^{\mathrm{prox}} u(x)| \\
&\overset{(d)}{\leq} \sum_{x\in\Omega} c_x \left(\Delta_A u(x)\right)^d \\
&\overset{(e)}{\leq} (\max_{x\in\Omega} c_x) \sharp\Omega \left(\frac{1}{\sharp\Omega} \sum_{(x,y)\in\overrightarrow{\partial\Omega}} g(x,y) \right)^d = \max_{x\in\Omega} c_x \frac{\left(\sharp_g \overrightarrow{\partial\Omega}\right)^d}{(\sharp\Omega)^{d-1}}.
\end{aligned}
$$

Generalization of arithmetic-geometric inequality:

$$|\partial^{\mathrm{prox}} u(x)| \leq c_x |\Delta_A u(x)|^d.$$

Main result – 1/2

Necessary conditions for equality:

- $c_x, x \in \Omega$ are all equal.
- $G|_{\overline{\Omega}}$ dual graph of a face-to-face decomposition of $\partial u(\Omega)$ into convex polyhedra of equal volume
- The PDI becomes a PDE (equality achieved).

Sufficient conditions for equality. (assume $\Omega \subset V$ connected in G).

- The complex made of vertices and edges of $G|_{\Omega} \cup \overrightarrow{\partial\Omega}$ is reciprocal to the collection of d- and $(d-1)$-cells of an equal-volume Voronoi tessellation of a convex polyhedron H.
- If $F_{x,y}$ denotes the $(d-1)$-dimensional facet of the Voronoi tessellation which is dual to edge (x, y) of G, then $\frac{A^2(x,y)|y-x|}{\mathcal{H}^{d-1}(F_{x,y})}$ takes the same value for all edges $\{x, y\}$ of G.

MAIN RESULT – 2/2

Relation to optimal transport

- Functions u achieving equality are precisely of the form $u = \lambda u_{\text{Alek}} + \ell$ where $\lambda > 0$, ℓ is an affine function and u_{Alek} is the Aleksandrov solution to a semidiscrete optimal transport problem between $\frac{|H|}{\sharp\Omega} \sum_{x\in\Omega} \delta_x$ and $1_H(x)dx$ with transport cost $|x-y|^2$.

The subdifferential optimization problem

Set $H_v(c) := \{p : v \cdot p \le c\}$ and for fixed $\mathcal{V} \subset \mathbb{R}^d$ we define

$$C_{\mathcal{V}} := \max \left\{ \left| \bigcap_{v\in\mathcal{V}} H_v(c_v) \right| : \vec{c} = (c_v)_{v\in\mathcal{V}} \in \mathbb{R}^{\mathcal{V}},\ \sum_{v\in\mathcal{V}} c_v = 1 \right\}.$$

- Optimizer exists iff $\text{Span}\mathcal{V} = \mathbb{R}^d$, $\sum_{v\in\mathcal{V}} v = 0$.
- The face F_v with normal v of the optimizer has area $d\, C_{\mathcal{V}} |v|$.

THE $\partial^{\mathrm{prox}} u(x)$-INEQUALITY

- We need $|\partial^{\mathrm{prox}} u(x)| \leq c_x (\Delta_A u(x))^d$ and discussion of equality case if $c_x, x \in \Omega$ all equal.
- Apply the above with $\mathcal{V}_x := \{(y-x)A^2(x,y) : \; y \sim x\}$, and then $c_x = C_{\mathcal{V}_x}$.
- We have

$$\frac{1}{\Delta_A u(x)} \partial^{\mathrm{prox}} u(x) = \bigcap_{v \in \mathcal{V}_x} H_v(c_v) \quad \text{with} \quad c_v = \frac{A^2(y,x)(u(y) - u(x))}{\Delta_A u(x)}.$$

- Equality case (assuming Ω connected): $|F_{x,y}|/(|y-x|A^2(x,y))$ constant over all edges.

Further connections/directions

- **Aurenhammer 1987, Rybnikov 1999**: translation between liftings, weighted Voronoi tessellations, reciprocal graphs.
- **Mérigot 2013, Benamou-Froese 2017**: link of the above to semidiscrete optimal transport.
- **Trudinger 1994**: further continuum isoperimetric inequalities (possible extension to operators of higher degree).
- Optimal discrete PDI in general graphs: first bounds in **Gomez-Petrache 2020**, general Cheeger type bounds to be explored.
- More complicated optimal inequalites in periodic graphs do exist (cf. triangular graph case above), classification missing.