Sharp discrete isoperimetric inequalities in periodic graphs via discrete PDE and Semidiscrete Optimal Transport

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(joint work in 2020 with Matías Gómez, who is now at Imperial College)

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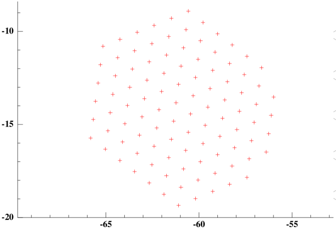
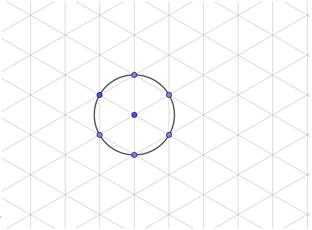
CRYSTAL STRUCTURES AND CLUSTER SHAPES

Example: $\min_{\{x_1,\ldots,x_N\}} \sum_{i\neq j} V(|x_i - x_j|)$, **Lennard-Jones** $V(r) = \frac{1}{r^{12}} - \frac{1}{r^6}$.

Numerics:



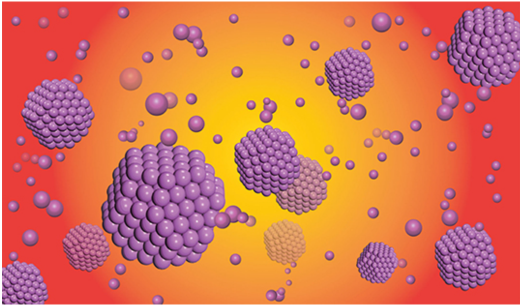


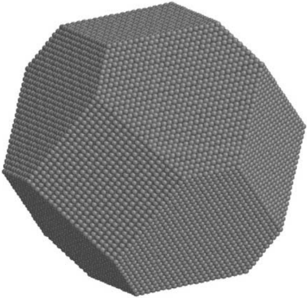
Local structure: triangular lattice.
Global shape: hexagon.

Tóth 1956, Heitmann-Radin 1980: sticky disk model.
Schmidt 2013: fluctuations around hexagon.
Theil 2006: triangular lattice crystallization

Bétermin-De Luca-Petrache 2019: crystal can be $\mathbb{Z}^2$ for soft sticky disc model (robust in V, limit $N \to \infty$). **Octagon shape**.

What other shapes? For which bond graphs?





ISOPERIMETRIC INEQUALITIES

Find $H \subset \mathbb{R}^d$ such that: $$\frac{\text{Area}(\partial H)^d}{\text{Vol}(H)^{d-1}} = \min_{\Omega \subset \mathbb{R}^d} \frac{\text{Area}(\partial \Omega)^d}{\text{Vol}(\Omega)^{d-1}}$$

- (Find best $C_H > 0$ such that $\text{Area}(\partial\Omega)^d \leq C_H \,\text{Vol}(\Omega)^{d-1}$.)
- Extended notion of "area", depending on norm g on normal vectors:

$$\text{Area}_g(\Omega) := \int_{\partial\Omega} g(\nu(x))dS(x).$$

Theorem (Wulff 1901)

For Vol *as usual and* Area_g *as above, optimizer is*

$$H = \{x \in \mathbb{R}^d : \forall \nu,\ x \cdot \nu < g(\nu)\},$$

up to dilation/rotation.

Discrete sharp isoperimetric inequality

Setup:

- $V \subset \mathbb{R}^d$ discrete set (allowed atom positions).
- $G = (V, E)$ undirected graph (bond graph).
- $g : E \to [0, +\infty)$ weight (boundary bond energies).

Looking for edge-isoperimetric inequalities of the form

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

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

Continuum isoperimetric proof – 1/3

Strategy 1: PDE + convexity

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

$$\begin{cases} \Delta u(x) = \frac{\text{Area}_g(\Omega)}{\text{Vol}(\Omega)} & x \in \Omega, \\ \frac{\partial u}{\partial \nu}(x) = g(\nu(x)) & x \in \partial\Omega. \end{cases}$$

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

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

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

Continuum proofs – 2/3

Claim: $H \subset \nabla u(\Gamma_u)$.

- $p \in H \overset{(def.)}{\Leftrightarrow} p \cdot \nu < g(\nu)$ whenever $|\nu| = 1$.
- Let $x \in \overline{\Omega}$ minimum of $u(y) - p \cdot y$.
- If $x \in \partial\Omega$ then $\frac{\partial(u(y)-p\cdot y)}{\partial \nu} \leq 0$..
  ..that is, $\frac{\partial u}{\partial \nu}(x) \leq p \cdot \nu$. Contradiction!
- So x is interior. It follows:
  - $p = \nabla u(x)$ (critical point),
  - $u(y) \geq u(x) + p \cdot (y - x), \forall y \in \overline{\Omega}$

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

We get $$\mathrm{Vol}(H) \leq \mathrm{Vol}(\nabla u(\Gamma_u)) = \int_{\nabla u(\Gamma_u)} dp \leq \int_{\Gamma_u} \det[D^2 u(x)] dx$$

CONTINUUM PROOFS – 3/3

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

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

We get $\mathrm{Vol}(H) \leq \mathrm{Vol}(\Gamma_u) \left(\frac{\Delta u(x)}{d}\right)^d$, **and then we have**:

$$\mathrm{Vol}(\Gamma_u) \leq \mathrm{Vol}(\Omega), \qquad \left(\frac{\Delta u(x)}{d} \right)^d = \left(\frac{\mathrm{Area}_g(\Omega)}{d \cdot \mathrm{Vol}(\Omega)} \right)^d .$$

We get

$$d^d \mathrm{Vol}(H) \leq \frac{\mathrm{Area}_g(\Omega)^d}{\mathrm{Vol}(\Omega)^{d-1}} .$$

Use that $g(\nu(x)) = x \cdot \nu(x)$ **on** ∂H **and divergence theorem:**

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

THE DISCRETE RESULT

- Auxiliary laplacian: $\Delta u(x) := \sum_{y:\{x,y\}\in E}(u(x) - u(y))$.
- Solve discrete PDI (discrete PDE not solvable in general)

$$\begin{cases} \Delta u(x) \leq \frac{\sharp_g \overrightarrow{\partial\Omega}}{\sharp\Omega} & \text{for } x \in \Omega \\ u(y) - u(x) = g(x,y) & \text{for } (x,y) \in \overrightarrow{\partial\Omega}. \end{cases}$$

- Subdifferential, proximal subdifferential, dual (Wulff) shape:

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

THE DISCRETE RESULT (GOMEZ-PETRACHE, ARXIV)

$$\mathrm{Vol}(H_g) \overset{(a)}{\leq} \mathrm{Vol}\left(\bigcup_{x\in\Omega} \partial u(x)\right) \overset{(b)}{=} \sum_{x\in\Omega} \mathrm{Vol}(\partial u(x)) \overset{(c)}{\leq} \sum_{x\in\Omega} \mathrm{Vol}(\partial^{\mathrm{prox}} u(x))$$

$$\overset{(d)}{\leq} \sum_{x\in\Omega} c_x \left(\Delta_A u(x)\right)^d \overset{(e)}{\leq} \left(\max_{x\in\Omega} c_x\right) \frac{\left(\sharp_g \overrightarrow{\partial\Omega}\right)^d}{(\sharp\Omega)^{d-1}}.$$

Crucial: "Minkowski" arithmetic-geometric inequality

$$c_x := \max\left\{\mathrm{Vol}\left(\bigcap_{v\in\mathcal{V}} H_v(c_v)\right) : \sum_{v\in\mathcal{V}} c_v = 1\right\},$$

where $\begin{cases} \mathcal{V} = \{y - x : \{x,y\} \in E\}, \\ c_v = \frac{u(y)-u(x)}{\Delta u(x)}. \end{cases}$

Then we get: $\mathrm{Vol}(\partial^{\mathrm{prox}} u(x)) \leq c_x(\Delta u(x))^d.$

We can add weights: $\Delta_W u(x) := \sum_{y\sim x} W(x,y)(u(y) - u(x))$.

THEOREM:

Necessary conditions on u, W, Ω for equality:

- *(Minkowski constants)* $(c_x)_{x\in\Omega}$ all equal,
- *(Subdifferential tiling)* $\partial^{\text{prox}}u(x), x \in \Omega$ equal volume partition of $\partial u(\Omega)$,
- *(Bond graph shape)* $G|_{\overline{\Omega}}$ reciprocal to the above partition,
- *(Convexity of Ω)* Our PDI achieves equality.

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

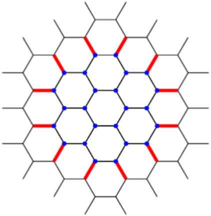
- The complex made of vertices and edges of $G|_{\Omega} \cup \overrightarrow{\partial\Omega}$ is reciprocal to the collection of d- and $(d-1)$-cells of an equal-volume Voronoi tessellation of a convex polyhedron H .
- $\exists W : E \to (0, +\infty)$ symmetric weight, such that $\frac{W^2(x,y)|y-x|}{\text{Area}(F_{x,y})}$ takes the same value for all edges $\{x, y\} \in E$, where $F_{x,y}$=facet dual to $\{x, y\}$.

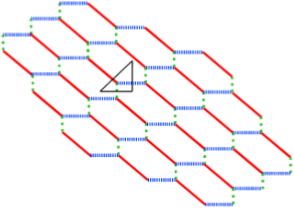
Link to optimal transport (Aleksandrov solutions):

- u achieves equality $\Leftrightarrow$ $u = \lambda u_{\text{Alek}} + \ell$ for some $\lambda > 0$, $\ell : \mathbb{R}^d \to \mathbb{R}$ affine, and
$$\partial u_{\text{Alek}} = \left[\text{Opt. Transp. of } \frac{\sum_{x\in\Omega} \delta_x}{\sharp\Omega} \text{ to } \frac{\mathcal{L}^d|_H}{\text{Vol}(H)}, \text{ under cost } |x-y|^2 \right].$$

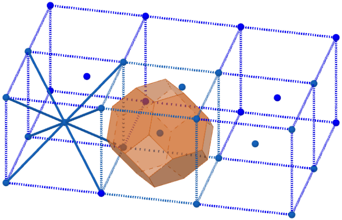
Examples:

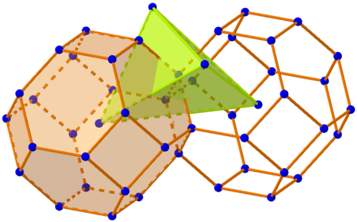
- Hexagons in Honeycomb graph, and deformations.





- Rhombic dodecahedra for skeleton of BCC.





THEOREM (CONSTRUCTION OF EXAMPLES):

- (tiling) Assume that we have an equal-volume tiling of $\mathbb{R}^d$ by convex sets.
- (alignment) The tiling is obtained by cutting $\mathbb{R}^d$ by hyperplanes.
- (reciprocal graph) Take the graph $G = (V, E)$ that is reciprocal to that tiling.
- Then we can find weight $W : E \to (0, +\infty)$ such that for an infinite family of Ω's in G the previous criterion shows that they are isoperimetric shapes.

(Examples: Coxeter hyperplane arrangements.)

Past results, unexplored directions:

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

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

    optimized only by "perfect hexagons"
    (follows by duality with honeycomb graph).

If you want to think about the problem:

- **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 (higher order operators / quermassintegrals).
- **Isoperimetric constant in graphs**: link to new(?) discrete laplacians in **Gomez-Petrache 2020**, general Cheeger type bounds to be explored.
- **Exotic forms of optimal inequalites in periodic graphs do exist**
  Continuum limit gives just leading order behavior
  $(\sharp\Omega)^{d-1} \leq C(\sharp_g \partial\Omega)^d$.
  Mystery: algebra behind the triangle graph case!