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High-dimensional node generation with variable density

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Fast Algorithms for
Generating Static and Dynamically Changing Point Configurations
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Joint work with
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Why discretize?

- Model network and sensor deployment.
- Data: storing smooth manifold as a discrete configuration.
- PDE solvers, radial basis functions interpolation etc. need well-distributed nodes.
- Additionally, the meshless methods often require non-uniform nodes.

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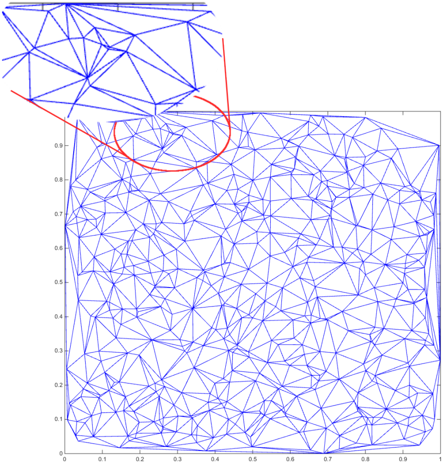
A bad example

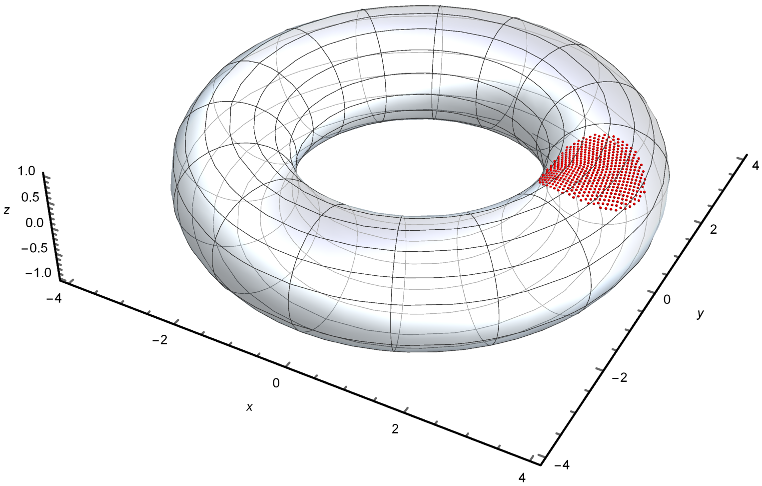
- (Uniform) random points exhibit clustering!



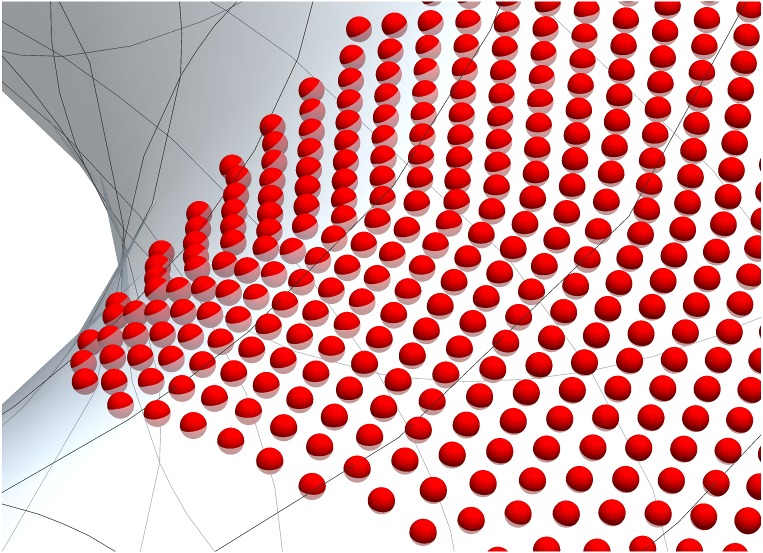
Delaunay triangulation of 500 uniformly random nodes in $[0,1]^2$.

A good example

Figure: 500 points, $s = 7,\ d = 2,\ q(x) = |x - x_0|^2$, where $x_0 := (3, 0, 1)^T$



Zoomed view



How to improve?

- sample from a distribution/process with repulsive properties
- apply thinning (to a Monte Carlo Markov chain)

  (still, neither of the above guarantees deterministic separation)

- Quasi-Monte Carlo methods
- Our suggestion: apply the gradient flow of a suitable functional to a suitable starting distribution

Weighted Riesz kernel

- $\mathcal{H}_d^A$ – normalized restriction of the d-dimensional Hausdorff measure
- $\omega_N = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\} \subset A$; $\tilde{\omega}_N$ – minimizers
- $E_s(\omega_N) := \sum_{\boldsymbol{x}\neq\boldsymbol{y}\in\omega_N} |\boldsymbol{x}-\boldsymbol{y}|^{-s}$, Riesz s-energy
- if $w(\cdot,\cdot)$ is $\mathcal{H}_d^A$-a.e. continuous on $A\times A$,

$$E_s(\omega_N; w) := \sum_{\substack{\boldsymbol{x}\neq\boldsymbol{y}\\ \boldsymbol{x},\boldsymbol{y}\in\omega_N}} \frac{w(\boldsymbol{x},\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|^s};$$

Theorem (Borodachov - Hardin - Saff, '14)

$s > d$ and $A \subset \mathbb{R}^p$ is d-rectifiable, compact, $\mathcal{H}_d(A) > 0$.
Every (asymptotically) minimal sequence $\{\tilde{\omega}_N\}_{N\geq 2}$ converges weak:*

$$\frac{1}{N}\sum_{\boldsymbol{x}\in\tilde{\omega}_N} \delta_{\boldsymbol{x}} \xrightarrow{*} \frac{1}{\mathcal{H}_d^{s,w}(A)} \cdot w^{-d/s}(\boldsymbol{x},\boldsymbol{x})\mathrm{d}\mathcal{H}_d^A \quad \text{as } N\to\infty.$$

($\mathcal{H}_d^{s,w}(A)$ is a normalizing constant) In particular, the asymptotics of the energy exists:

$$\lim_{N\to\infty} \frac{E_s(\tilde{\omega}_N; w)}{N^{1+s/d}} = \frac{C_{s,d}}{\mathcal{H}_d^{s,w}(A)^{s/d}}.$$

External field

- $q : A \to (\infty, \infty]$ – lower semi-continuous function
- For $s > d$, (s, d, q)-energy is

$$E_s(\omega_N; q) := \sum_{\substack{\boldsymbol{x} \neq \boldsymbol{y} \\ \boldsymbol{x}, \boldsymbol{y} \in \omega_N}} |\boldsymbol{x} - \boldsymbol{y}|^{-s} + N^{s/d} \sum_{\boldsymbol{x} \in \omega_N} q(\boldsymbol{x}).$$

- constant $M_{s,d} := (C_{s,d}(1 + s/d))^{-d/s}$

Theorem (Hardin - Saff - V, '16)

Take A, s as in the BHS-theorem. Every (asymptotically) minimal sequence $\{\tilde{\omega}_N\}_{N\geq 2}$ converges weak:*

$$\frac{1}{N}\sum_{\boldsymbol{x}\in\tilde{\omega}_N}\delta_{\boldsymbol{x}} \xrightarrow{*} M_{s,d}\,(L_1-q)_+^{d/s}\,\mathrm{d}\mathscr{H}_d^A =: \mathrm{d}\mu_q \quad \textit{as } N\to\infty.$$

In particular, the asymptotics of the energy exists:

$$\lim_{N\to\infty}\frac{E_s(\tilde{\omega}_N;q)}{N^{1+s/d}} = \mathfrak{S}(q,A),$$

where

$$\mathfrak{S}(q,A) := \int \frac{L_1 d + q(\boldsymbol{x})s}{d+s}\,\mathrm{d}\mu_q(\boldsymbol{x}).$$

The $L_1 = L_1(q,A)$ is the (unique) constant such that $\mathrm{d}\mu_q$ is a probability measure on A.

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(Re)Producing a distribution

Given an upper semi-continuous $\rho : A \to [0, \infty)$ such that $\rho \, \mathrm{d}\mathscr{H}_d^A$ – probability measure, define

$$w(\boldsymbol{x}, \boldsymbol{y}) := (\rho(\boldsymbol{x})\rho(\boldsymbol{y}) + |\boldsymbol{x} - \boldsymbol{y}|)^{-s/2d}, \quad \text{and} \quad q(\boldsymbol{x}) := -\left(\frac{\rho(\boldsymbol{x})}{M_{s,d}}\right)^{s/d}.$$

Any sequence $\{\tilde{\omega}_N\}_{N\geq 2}$ minimizing either

$$E_s(\omega_N; w) = \sum_{\substack{\boldsymbol{x} \neq \boldsymbol{y} \\ \boldsymbol{x}, \boldsymbol{y} \in \omega_N}} \frac{w(\boldsymbol{x}, \boldsymbol{y})}{|\boldsymbol{x} - \boldsymbol{y}|^s}$$

or

$$E_s(\omega_N; q) = \sum_{\substack{\boldsymbol{x} \neq \boldsymbol{y} \\ \boldsymbol{x}, \boldsymbol{y} \in \omega_N}} |\boldsymbol{x} - \boldsymbol{y}|^{-s} + N^{s/d} \sum_{\boldsymbol{x} \in \omega_N} q(\boldsymbol{x}).$$

converges to $\rho \, \mathrm{d}\mathscr{H}_d^A$, $N \to \infty$.

Kernel truncation

- Turns out, one may assume $w(\cdot,\cdot) = w_N(\cdot,\cdot)$ satisfies

$$w(\boldsymbol{x},\boldsymbol{y}) = 0, \quad \text{if} \quad |\boldsymbol{x}-\boldsymbol{y}| > r_N,$$

  where

$$r_N \to 0 \quad \text{so that} \quad r_N N^{1/d} \to \infty.$$

  that is, outside an r_N-neighborhood of $\operatorname{diag}(A \times A)$
- this does not change the limiting measure
- we call this modification the truncated Riesz kernel.
- applies to the $E(\omega_N; q)$ energy as well
- in practice, for a fixed range of N it suffices only to take into account several nearest neighbors

Family of energies

$$E_s(\omega_N; w, q) = \sum_{\substack{\boldsymbol{x} \neq \boldsymbol{y} \\ \boldsymbol{x}, \boldsymbol{y} \in \omega_N}} \frac{w(\boldsymbol{x}, \boldsymbol{y})}{|\boldsymbol{x} - \boldsymbol{y}|^s} + N^{s/d} \sum_{\boldsymbol{x} \in \omega_N} q(\boldsymbol{x}).$$

- flexibility in choosing the functional
- the cost of evaluation of the density defines the costs of w and q
- local forces in w vs global in q

Short-scale properties of minimizers

- Optimal order of minimal pairwise distances, $N^{-1/d}$, for $s > d$.
- Under mild smoothness assumptions minimizers have the optimal covering radius of order $N^{-1/d}$ on any sublevel set $A(u)$ for all $u < L_1$.
- For $d \geq 2$, and $s > d$, the value of constant $C_{s,d}$ is known only numerically. Still, the distribution is stable under small perturbations of the value of $C_{s,d}$.

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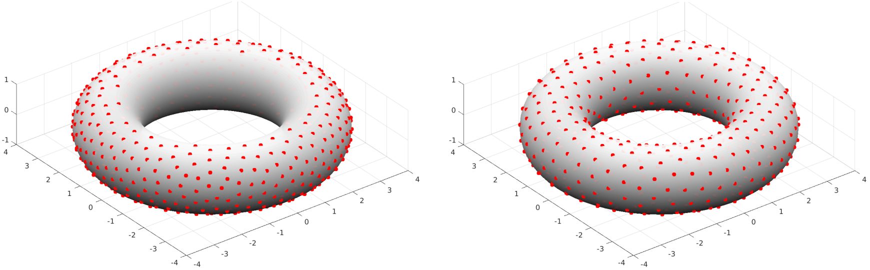
Restriction $s > d$ is important

Let A – torus, $\dim A = 2$,



are 500-point approximate minimizers. Left: $s = 0.5$; right: $s = 4$.
This is an artifact of using the ambient, not geodesic, distance.

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Gradient dynamics and its initialization

- Picking a random starting position slows down the optimization.
- The hypersingular kernel is short-ranged; let us try a locally suitable starting set, then apply minimization.
- For Monte Carlo methods piecewise distribution generation: *stratification*.
- Since we prohibit clustering, let's use quasi-Monte Carlo on individual pieces.

Gradient flow

- $\boldsymbol{x}_{j(i,k)}^{(t)}$ – nearest neighbors to $\boldsymbol{x}_i^{(t)}$, $1 \leq k \leq K$; $\Delta\left(\boldsymbol{x}_i^{(t)};\ \omega_N^{(t)}\right)$ – distance to the nearest neighbor
- Perform T iterations, moving in the direction of vector $\boldsymbol{g}_i^{(t)}$:

$$\boldsymbol{g}_i^{(t)} = -\nabla_i E_s\left(\left\{\boldsymbol{x}_{j(i,k)}^{(t)}\right\};w\right) \quad 1 \leq i \leq N.$$

- $C > 0$, constant

$$\boldsymbol{x}_i^{(t+1)} = \begin{cases} \boldsymbol{x}_i^{(t)} + \dfrac{1}{t+C} \cdot \Delta\left(\boldsymbol{x}_i^{(t)};\ \omega_N^{(t)}\right) \cdot \dfrac{\boldsymbol{g}_i^{(t)}}{\|\boldsymbol{g}_i^{(t)}\|} & \text{if this sum is inside } A; \\ \boldsymbol{x}_i^{(t)}, & \text{otherwise.} \end{cases}$$

- $\approx$ truncated Langevin dynamics $\implies$ considered in the math.phys. community, Chafaï et al, Duerinckx, Serfaty, etc.

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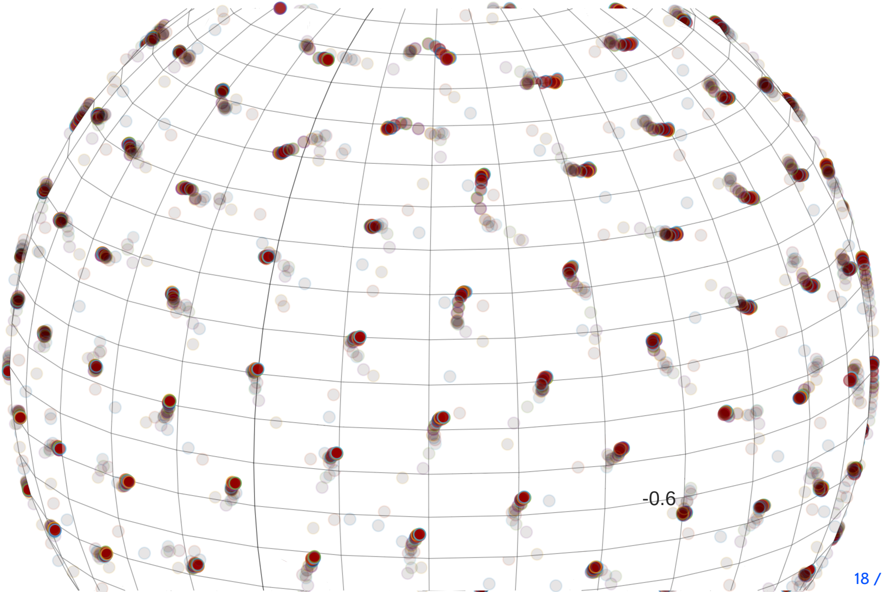
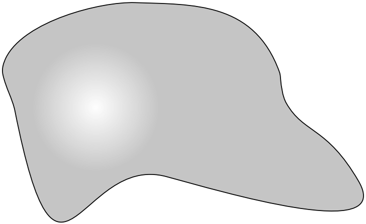
Dynamics illustration

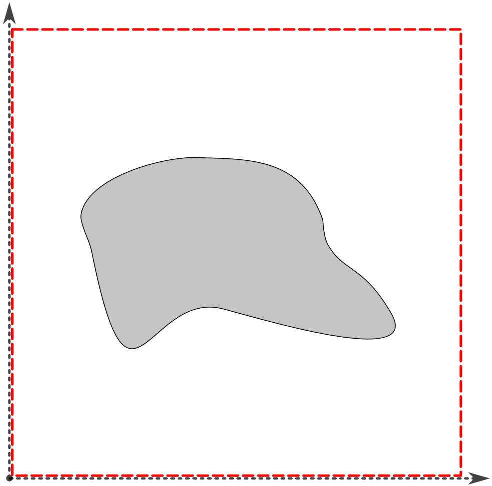
200 spherical points



Algorithm (Flyer - Fornberg - Michaels - V, '17)

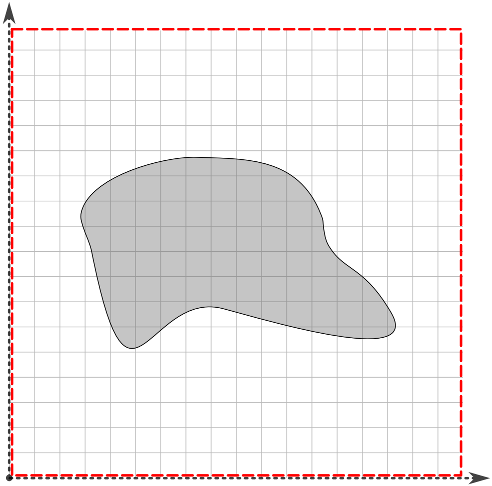


Algorithm (Flyer - Fornberg - Michaels - V, '17)



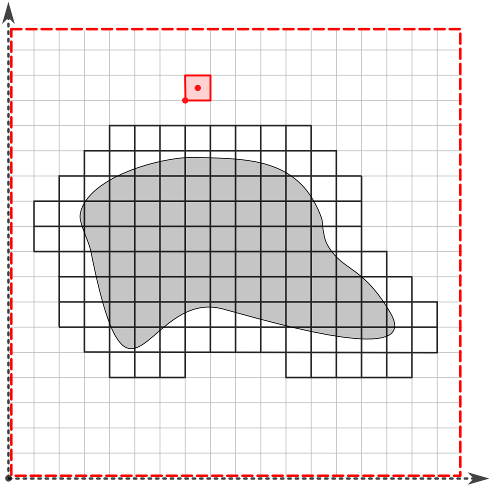
Algorithm (Flyer - Fornberg - Michaels - V, '17)

- partition the domain using a uniform (or adaptive) grid



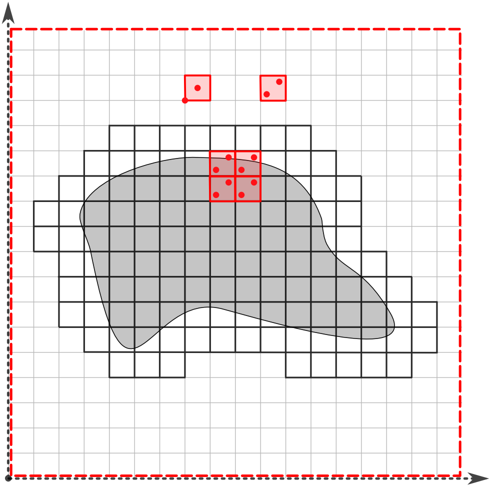
Algorithm (Flyer - Fornberg - Michaels - V, ’17)

- detect support; use only the cells close to it



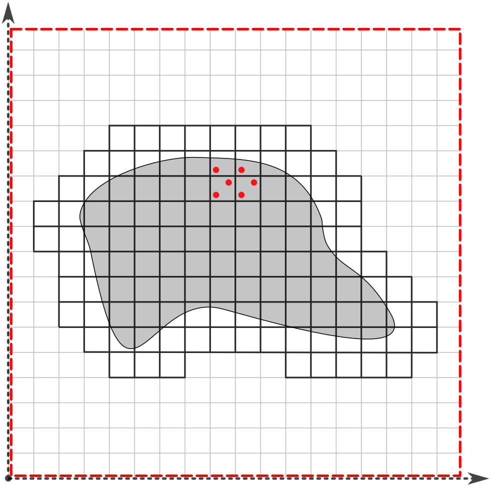
Algorithm (Flyer - Fornberg - Michaels - V, '17)

- place rescaled/translated/otherwise adapted pieces in each cell



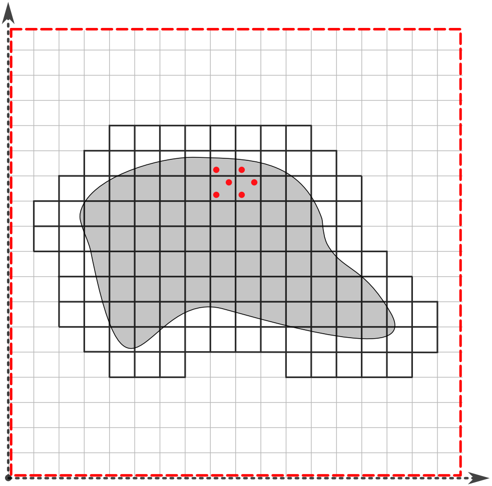
Algorithm (Flyer - Fornberg - Michaels - V, '17)

- make sure no points are outside the support



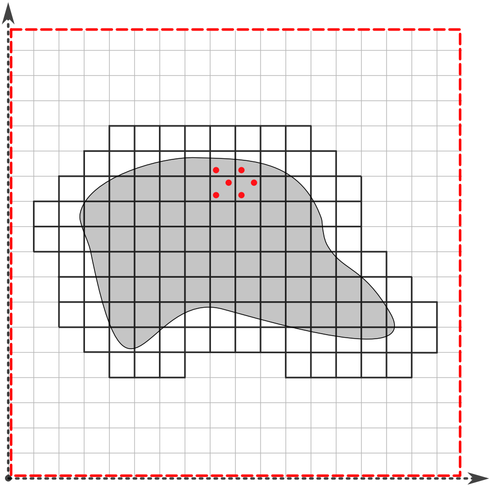
Algorithm (Flyer - Fornberg - Michaels - V, '17)

- apply the gradient flow, weighted with the desired density



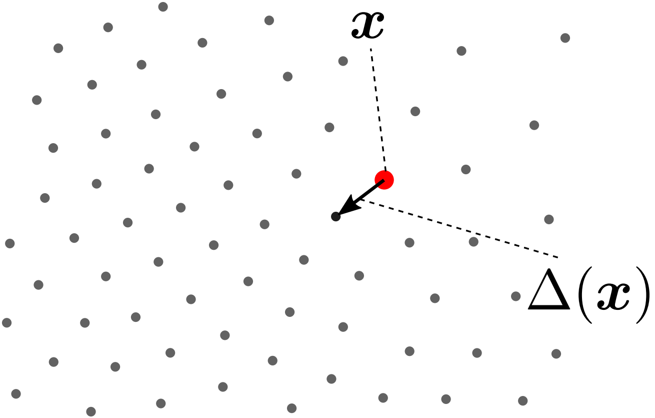
- fill the sparser parts of the distribution by *saturation*

(’greedy’ procedure, conceptually similar to bubble packing by Shimada)



Modified question

Distance from a node to the nearest neighbor has to be approximately equal to a given function of its position: $\Delta(\boldsymbol{x}) \approx \rho(\boldsymbol{x})$



We call ρ the *radial density*. Note: it is Lipschitz-1.

Modified algorithm

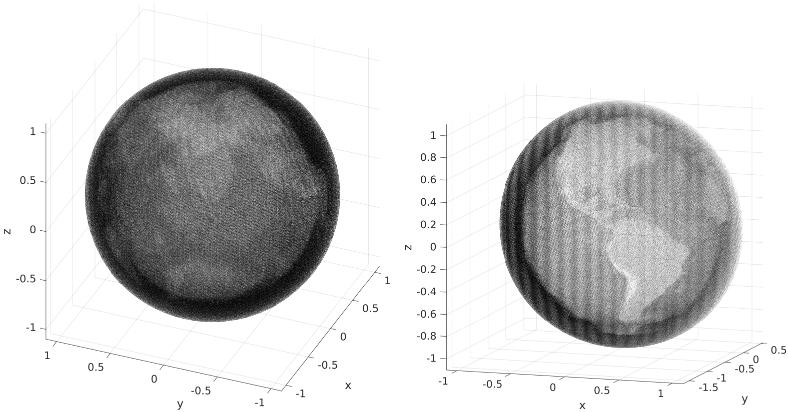
...

- place rescaled/translated/otherwise adapted pieces in each cell
    1. tabulate separation for a pre-determined node sequence (Riesz minimizers or ILs)
    2. use appropriate number of nodes, according to the desired separation
    3. transition between the multiplicative weight and radial density is governed by $w \asymp \Delta^s,\ N \to \infty$

...

Earth surface

- Goal: regularity on complex surfaces for the uniform density.
  An atmospheric layer with faithful surface recovery:



$\approx 1.35M$ nodes, generated in ≈ 3 minutes using ETOPO1 surface data and ray-tracing inclusion algorithm. The $\mathscr{L}_n$ lattice parameters $\alpha_1 = \sqrt{2}$, $\alpha_2 = (\sqrt{5}-1)/\sqrt{2}$.

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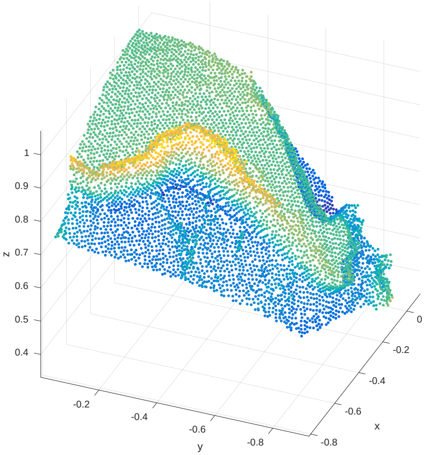
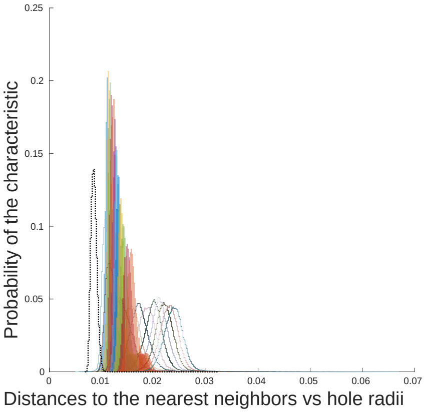
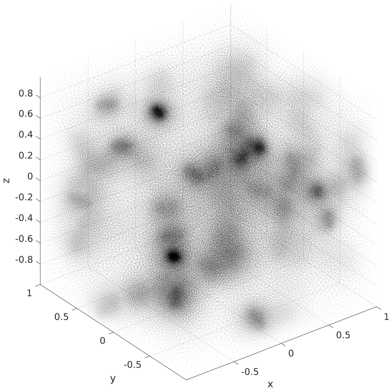
Earth surface: Andes

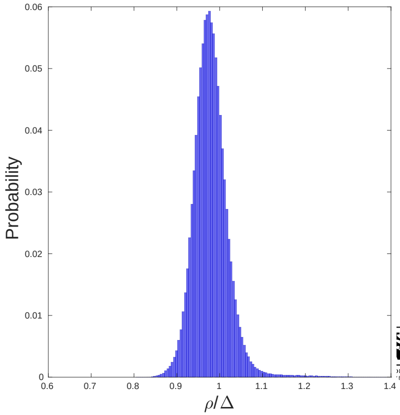




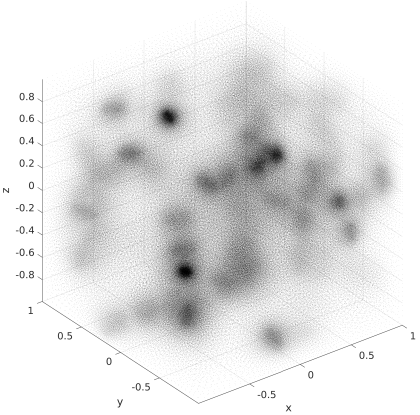
Point cloud

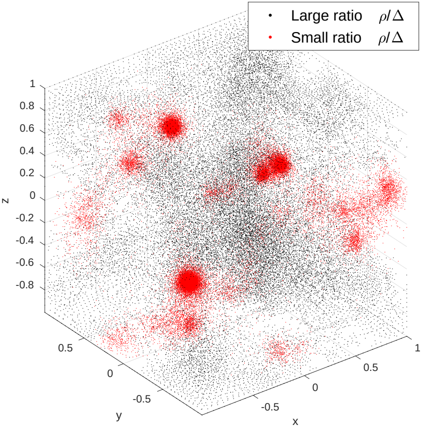
- Random 100 points $\mathscr{P}_{100}$ inside $[-1,1]^3$. Consider the radial density:
$$\rho(\boldsymbol{x}) = \left(\Delta(\boldsymbol{x};\mathscr{P}_{100}) + \Delta^2(\boldsymbol{x};\mathscr{P}_{100})\right)/20,$$
where Δ^2 for the distance to the 2-nd nearest neighbor.
- Goal: density recovery. Output: Left: 577,321 nodes; 200 interations of flow stepping in $\approx$ 12 minutes . Right: ratio of target/actual densities.





Point cloud: error location



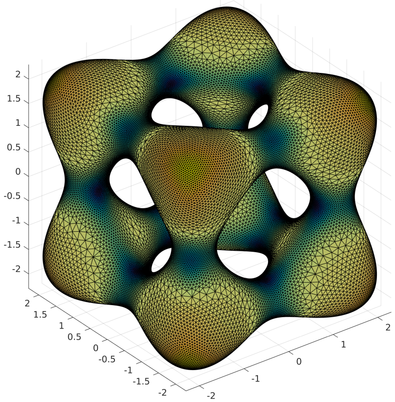


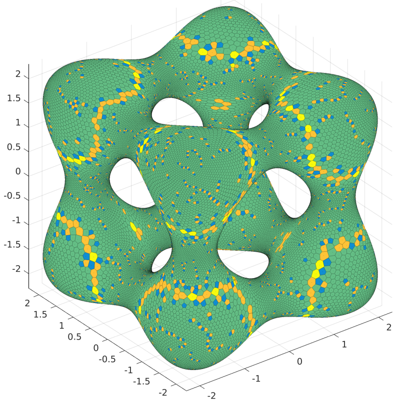
Surface Voronoi

- Chmutov-Banchoff-type surface:

$$x^2(x^2-5)+y^2(y^2-5)+z^2(z^2-5)+11=0$$

- 40K points distributed according to the absolute value of the Gaussian curvature. Left: color-coded Gaussian curvature, blue/orange is lower/higher. Right: surface Voronoi diagram.





Candidates for Quasi-Monte Carlo initialization

- irrational lattices (easy to generate, scalable)
  Pick $\alpha_1, \ldots, \alpha_{d-1}$ linearly independent over $\mathbb{Q}$, fix $0 < \delta < 1$

$$\mathscr{L}_n := \left\{ \left(\left\{ \delta + \frac{i}{n} \right\}, \{i\alpha_1\}, \{i\alpha_2\}, \ldots, \{i\alpha_{d-1}\} \right) \right\}_{i=1}^{n}$$

  $\{x\} \equiv x \bmod 1.$

  1. $\mathscr{L}_n$ weakly converge to the uniform distribution
  2. pointwise separation depends on the "irrationality properties" of $\alpha_1, \ldots, \alpha_{d-1}$, apparently on the continued fraction approximation
  3. *Korobov point sets* for the Q-MC community; *Kronecker sequences* for number theorists; *IL* is the low-discrepancy term.

- periodic Riesz minimizers (optimal filling)

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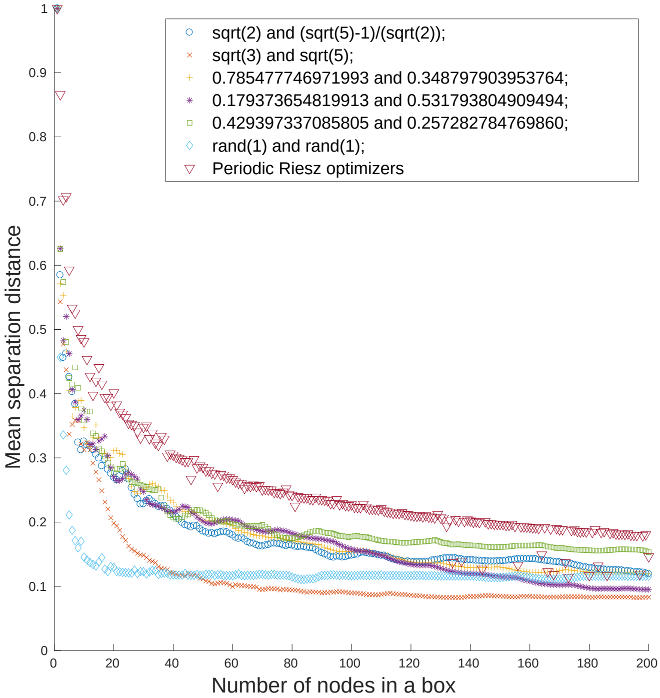
Separation of ILs: a curiosity



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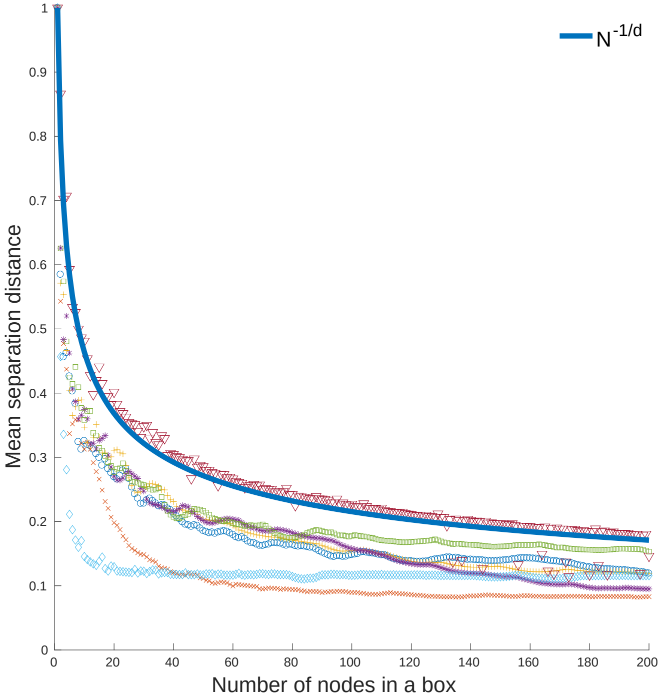

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Implementation

- Matlab prototype; uses the default knn.
  - https://github.com/OVlasiuk/3dRBFnodes
  - https://github.com/OVlasiuk/BRieszk
- Efficient for small to medium scales.

Conclusion

- Riesz energy-based functionals for construction of sets with a predefined density, volumetric and related
- suitable for meshless methods
- parallelizable
- reliably attains optimal separation
- practically suitable for tessellating (2d surfaces)
- (almost) dimension-agnostic
- allows modest (in terms of Wasserstein distance) distribution updates

- on large scales the singularity can cause precision loss, mitigated by smoothing
- relies on finding nearest neighbors

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Thank you!

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