Exploring 2D shape space: the hunt for the densest RSA packings

Konrad Kozubek[1] Piotr Kubala[1] Michał Cieśla[1] Adrian Baule[2]

[1]Institute of Theoretical Physics, Department of Statistical Physics, Jagiellonian University, Łojasiewicza 11, 30-348 Kraków, Poland

[2]School of Mathematical Sciences, Queen Mary University of London, London E1 4NS, United Kingdom

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- Methodology of the search for a shape maximizing saturated RSA packing fraction

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- Results of the numerical study and their discussion

Presentation outline

1. Random sequential adsorption

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Random sequential adsorption (RSA)

Definition of random sequential adsorption

Random sequential adsorption is a mathematical model of creation of unordered packings.
One iteration of the RSA algorithm:

- sample position and orientation of a trial particle from the uniform distribution;
- if the trial particle intersects with any of the previously added particles, discard it;
- otherwise add the trial particle to the packing and keep its position and orientation unchanged.

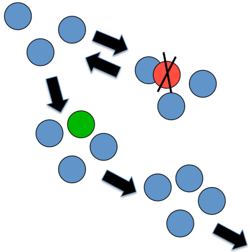

Figure 1: Visualisation of two steps of the RSA algorithm

RSA packing is saturated, if adding a particle to it is impossible.

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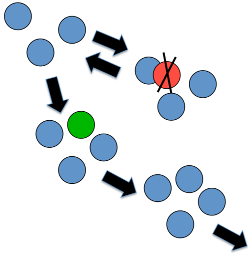

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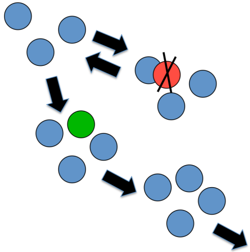

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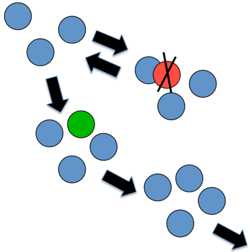

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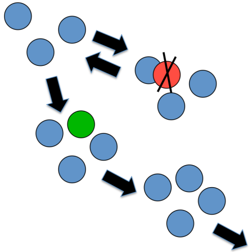

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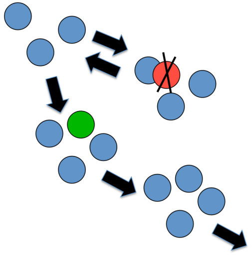

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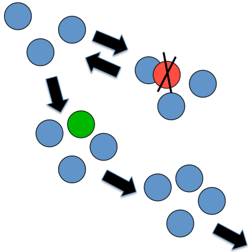

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Applications of RSA

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2. Analysis of properties of unordered packings – a simple model with excluded volume effects

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Properties of RSA

- For appropriate types of packing spaces and particles *packing fraction* can be defined
- *Kinetics* – mean rate of growth of the packing
- Power law governing kinetics:

$$\theta(t) = \theta - At^{-1/d}, \tag{1}$$

where $\theta(t)$ and θ – mean packing fractions after t iterations and at saturation, $A > 0$ i d – constants, $t \gg 1$ [1].

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Two methods of estimation of saturated packing fraction

Goal: for a given particle shape and packing space estimate the mean saturated packing fraction θ.

Methods of packing fraction estimation:

1. Estimation based on RSA kinetics
2. Generation of saturated packings

Algorithms for generation of saturated RSA packings exist among others for polydisks [2] and rounded polygons [3].

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Search for a shape maximizing saturated packing fraction

Goal: find a 2-dimensional shape forming 2-dimensional RSA packings with maximal mean saturated packing fraction.

Previous searches for a shape forming the densest RSA packings were limited to a few classes of basic shapes, for example (smoothed) dimers of different anisotropies [4] and linear *n*-mers, diskorectangles and ellipses of different anisotropies [5]. Only in a few studies saturated packings were generated.

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Search for a shape maximizing saturated packing fraction

shape type	anisotropy	packing fraction
disk [6]	1	0.547 073 5(28)
rectangle [7]	1.492(22)	0.549 632(17)
dimer [2]	1.5	0.577 658(17)
smoothed dimer [4]	1.6347	0.5833(5)
diskorectangle [8]	1.84	0.582 896(19)
ellipse [8]	1.84	**0.583 999(17)**

Table 1: Chosen previous searches for shapes giving high packing fractions

[6] G. Zhang and S. Torquato, *Physical Review E* 88.5 (2013), p. 053312.

[7] W. Kasperek, P. Kubala, and M. Cieśla, *Physical Review E* 98.6 (2018), p. 063310.

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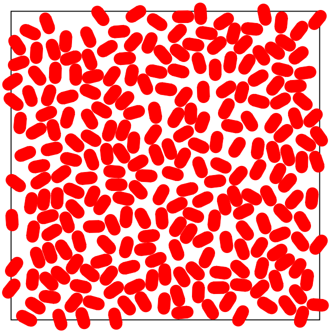

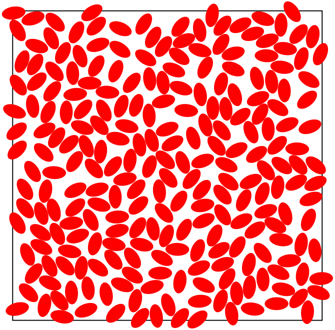

(a) (b)

Figure 2: Saturated RSA packings of diskorectangles (a) and ellipses (b) of anisotropy 1.84. Packing fractions: 0.6 (a), 0.605 (b), mean saturated packing fractions: 0.582 896(19) (a), 0.583 999(17) (b) [8].

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Exploring shape space – shape optimization

Shape space – set of all sensible 2-dimensional shapes forming RSA packings.
In this study, a different approach is used – larger subspaces of shape space are explored to find the best shapes. Search uses two things:

1. a conveniently parametrized subspace of shape space (for example polydisks)
2. and a convenient optimization algorithm.

Similar study was performed for shapes built of overlapping 3-dimensional balls, forming jammed packings under influence of gravity [9]. It showed that CMA-ES algorithm is convenient for such kind of problems.

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Covariance Matrix Adaptation Evolution Strategy (CMA-ES)

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It is an *evolutionary algorithm* – it uses mechanisms inspired by biological evolution: reproduction, mutation, recombination, and selection.

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Initialize distribution parameters $\varphi^{(0)}$;
$g \leftarrow 0$;
while *termination condition is not met* **do**
    Sample λ independent points $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_\lambda$ from distribution $p(\boldsymbol{x}; \varphi^{(g)})$;
    Evaluate f on samples;
    Update distribution parameters: $\varphi^{(g+1)} \leftarrow F(\varphi^{(g)}, (\boldsymbol{x}_1, f(\boldsymbol{x}_1)), (\boldsymbol{x}_2, f(\boldsymbol{x}_2)), \ldots, (\boldsymbol{x}_\lambda, f(\boldsymbol{x}_\lambda)))$;
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Algorithm 1: CMA-ES [10].

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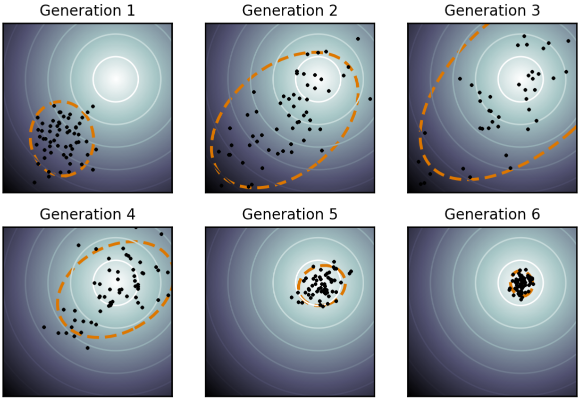

Figure 3: Illustration of CMA-ES algorithm run in 2-dimensional space[1].

[1] https://commons.wikimedia.org/wiki/File:Concept_of_directional_optimization_in_CMA-ES_algorithm.png

CMA-ES properties

- Black-box optimization
- Low number of evaluations
- Good performance in high dimensions
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Optimization schema

$$
\begin{tikzcd}
\mathbb{R}^n \arrow[r, bend left, "f_{\mathrm{sp}}"] \arrow[rrr, bend right, "f"] & \mathbb{S}_{\mathrm{p}} \subset \mathbb{R}^m \arrow[r, bend left, "f_{\mathrm{s}}"] & \mathbb{S} \arrow[r, bend left, "f_{\mathrm{spf}}"] & {[0,1]}
\end{tikzcd}
$$

optimization space

shape parameters space

subspace of shape space

packing fraction space

Figure 4: Optimization schema

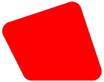
Optimization schema – example

$$(-0.5, 3, 2, 3, -1, 4)$$

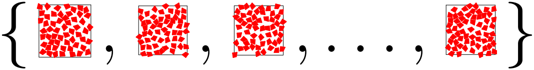
$$\Big\downarrow f_{\mathrm{sp}}$$

$$(\underbrace{\ln(1+\exp(-0.5))}_{0.474\ldots}, (0,0), (0,3), (2,3), (-1,4))$$

$$\Big\downarrow f_{\mathrm{s}}$$



$$\Big\downarrow f_{\mathrm{p}}$$



$$\Big\downarrow f_{\mathrm{pf}}$$

$$0.5768(20)$$

Figure 5: Optimization schema – example

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Polydisk optimization

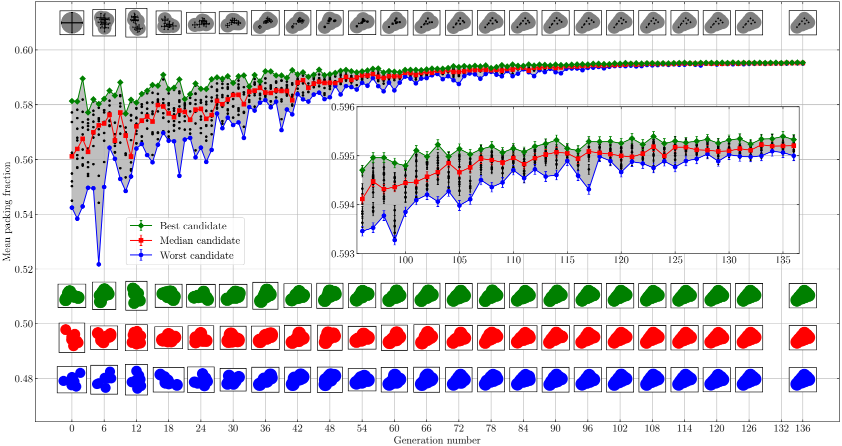


Figure 6: Illustrative optimization of a fixed-radii, connected 9-disk using CMA-ES optimization. Black dots correspond to the mean saturated packing fraction of particular shapes in generations. The green, red, and blue dots correspond to the best, the median and the worst candidates, respectively, in the population. The gray shapes above correspond to the center of the probability distribution used by the CMA-ES algorithm.

Rounded polygon optimization

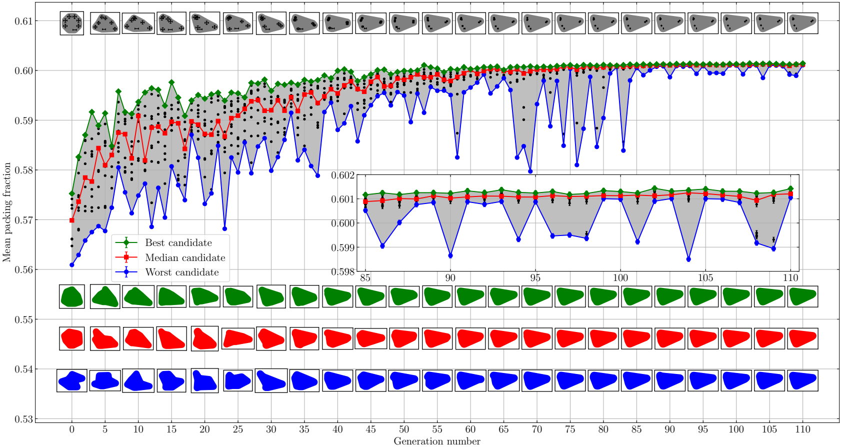
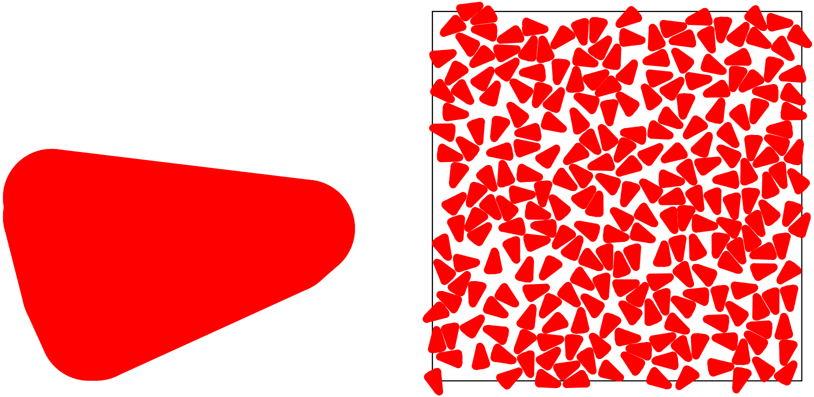


Figure 7: Illustrative optimization of a rounded, fixed-radius 8-gon using CMA-ES optimization. Black dots correspond to the mean saturated packing fraction of particular shapes in generations. The green, red, and blue dots correspond to the best, the median and the worst candidates, respectively, in the population. The gray shapes above correspond to the center of the probability distribution used by the CMA-ES algorithm. Best packing fraction: 0.601 43(10).

Current results of the search



(a) (b)

Figure 8: (a) Shape giving the highest RSA packing fraction so far – rounded 8-gon. (b) Saturated RSA packing of the best "triangular" shape of packing fraction 0.6275. Mean saturated packing fraction: 0.601 43(10).

Literature and further reading

[1] J. Feder, "Random sequential adsorption", *J. Theor. Biol.* **87**.2 (1980), pp. 237–254.

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The end

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