Network models of biological structures

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Abstract:

Random biological structures (sets of bacteria, biological tissue, sets of cells etc) can be considered as random two-phase geometric structures described by probabilistic distributions, for instance, by correlation functions. This talk is devoted to a new computationally effective approach for the representative volume element (RVE) based on the so-called e-sums (multidimensional discrete chain convolutions). The e-sums contain geometric statistical information hidden in the considered structures when interactions between particles of various physical phenomena such as viscous, elastic stresses and deformations, diffusion, heat, electric and magnetic fields occur. We compare two samples which are not statistically distinguishable at the first glance.
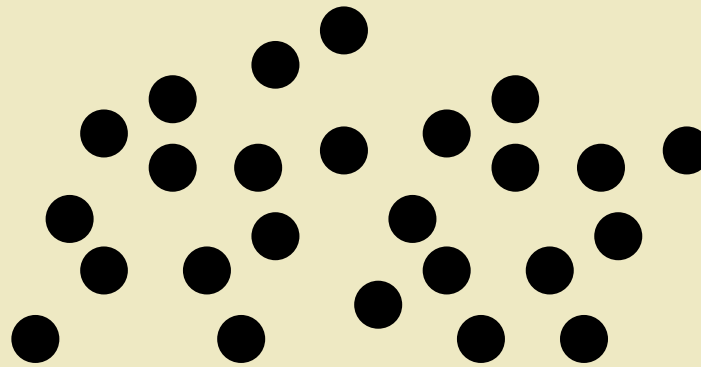
Mityushev V., Pattern formations and optimal packing, Mathematical Biosciences 2016

Czapla R., Mityushev V., A criterion of collective behavior of bacteria, Mathematical Biosciences and Engineering, 2017

Mityushev V., Optimal and stable random pattern formations J Theoretical Biology 2017

S. Gluzman, V. Mityushev, W. Nawalaniec, Computational Analysis of Structured Media (will be published in October 2017, Elsevier)

Computational Analysis of Structured Media

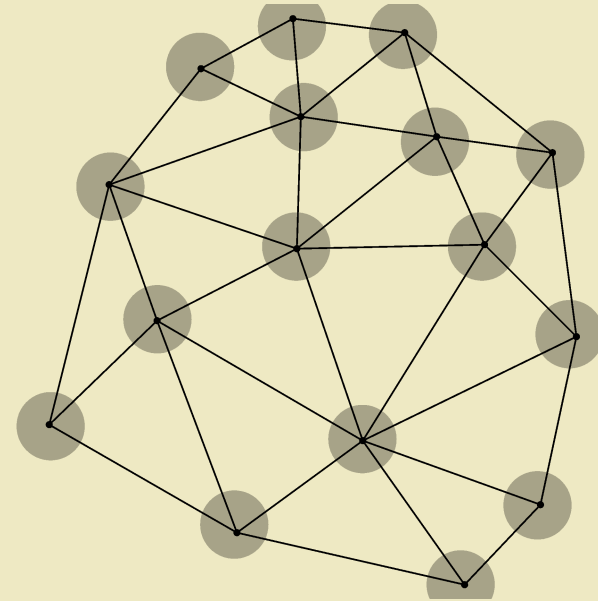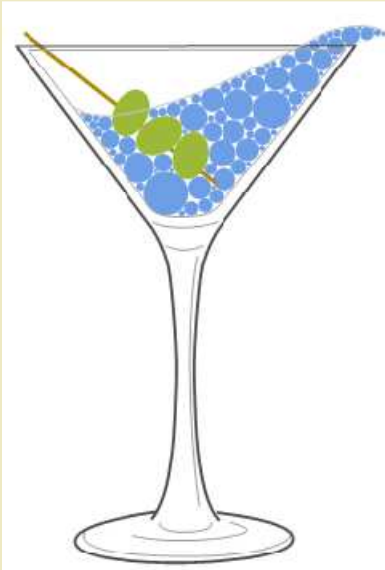Simon Gluzman,
Vladimir Mityushev,
and Wojciech Nawalaniec
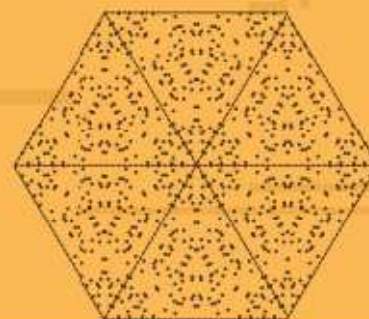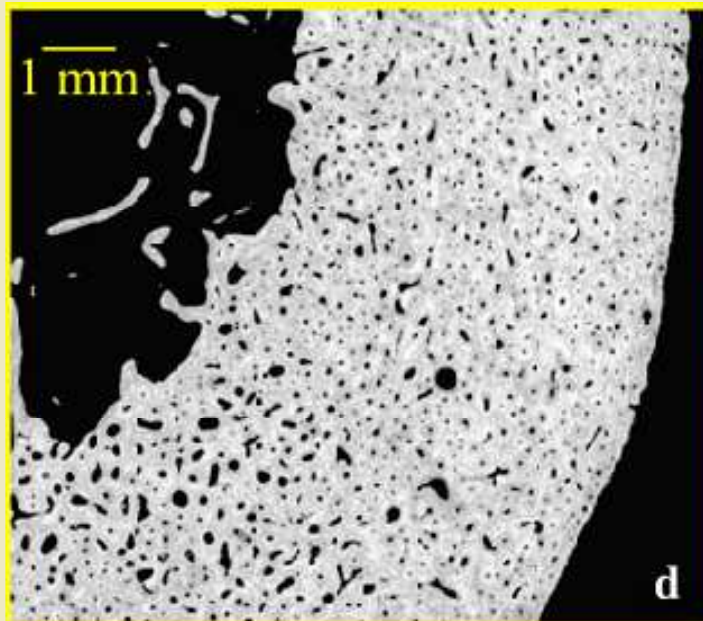
Mathematical Analysis and its Applications

Series Editor
Themistocles M. Rassias

Why did James Bond prefer shaken, not stirred martini with ice?
Transformation of dispersed structure to a Delaunay graph

❑   *Typical empirical and theoretical investigation:* **Microstructure of the human bone (MKH Malo, D Rohrbach, H Isaksson, J Töyräs, JS Jurvelin, IS Tamminen, 2013)**


Femoral neck and shaft in tissue; porous medium

Mathematical modeling is based on the structure of local fields (elastic, thermal, electric, magnetic, viscous etc) and the macroscopic constants.

We are interested in the passage from a single object to interactions between randomy distribued objects.

Example: from one bacterium to self-organization and collective behavior of bacteria
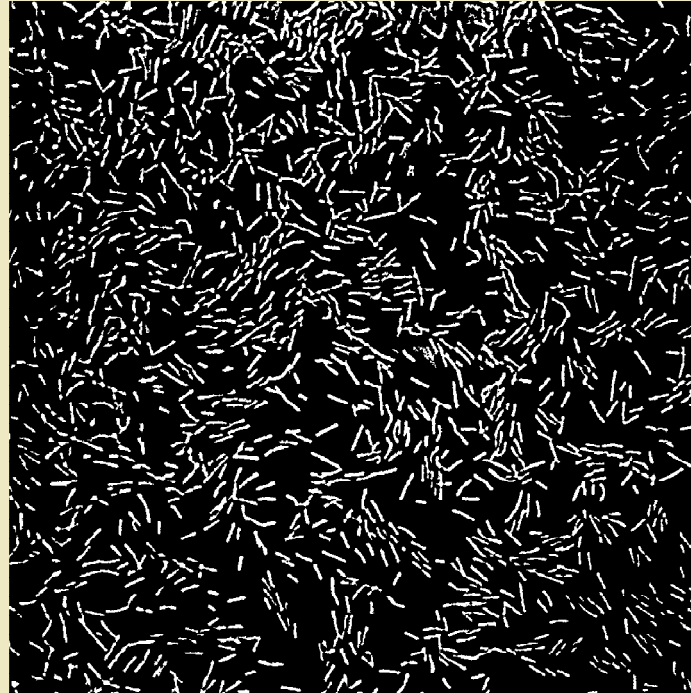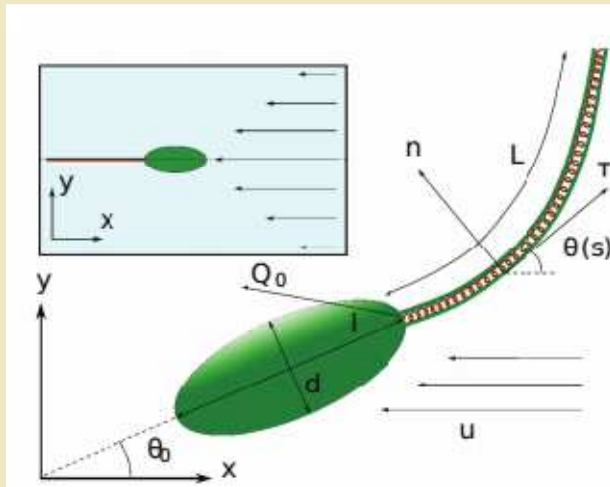
a) Due to M. Tournus, A. Kirshtein, L.V. Berlyand, and I.S. Aranson (J Roy Soc Interface 2015)
b) Due to S. D. Ryan, A. Sokolov, L. Berlyand and I.S. Aranson (New Journal of Physics 2013)
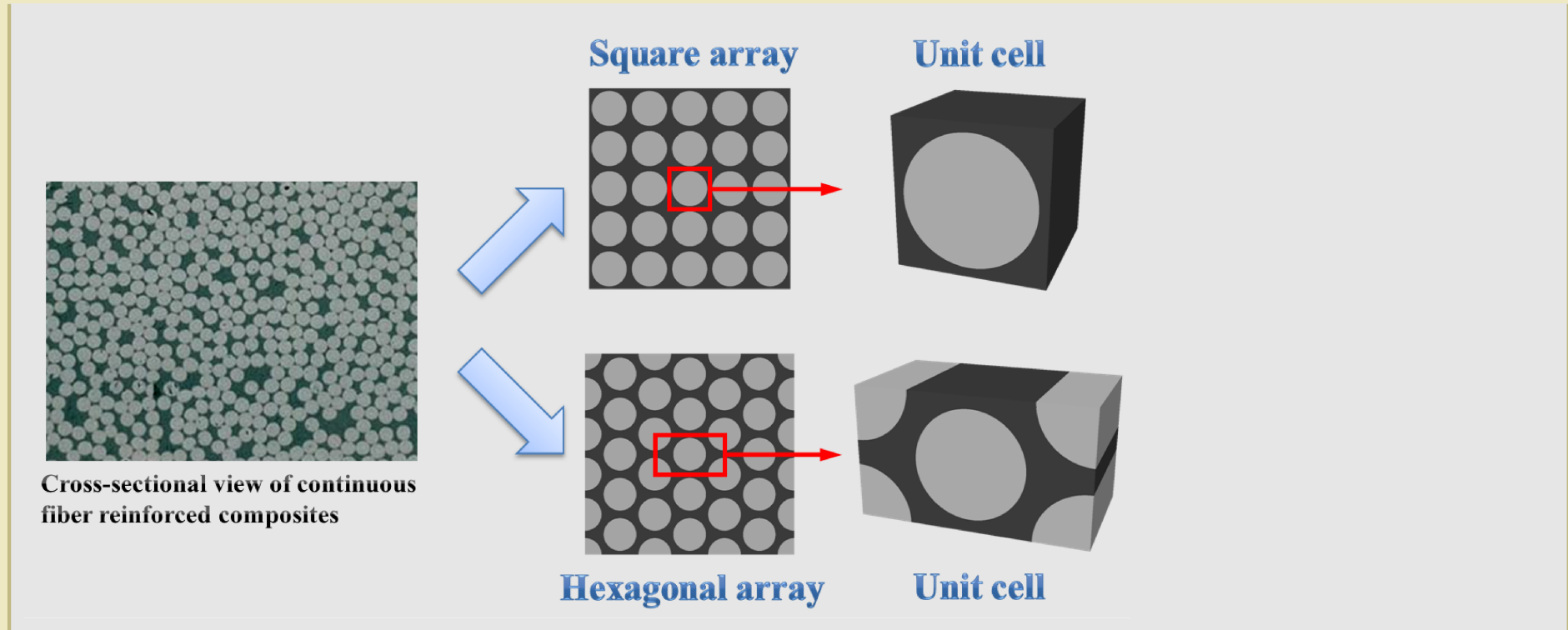
"Theorem":
The macroscopic constants are determined by means of the geometry.
RVE (representative volume element) determined the geometry.

The main question: how to describe the geometry and identify its features?

Applications: how to distinguish healthy and ill bio structures? how to distinguish their dynamic features?

■ **Traditional Scheme of the RVE from WikipediA**

Square array   Unit cell

Cross-sectional view of continuous
fiber reinforced composites

Hexagonal array   Unit cell

Contradict to the extremality principle of regular structures, see Berlyand L., Mityushev V. (J Statist. Phys. 2001, 2005)

Corellation functions

Direct description of random media by n- point corellation functions [Beran (1968), Torquato (2001)]:

1 - point corellation function (concentration);

2 - point corellation functions $S_2(r)$ (autocorellation) etc
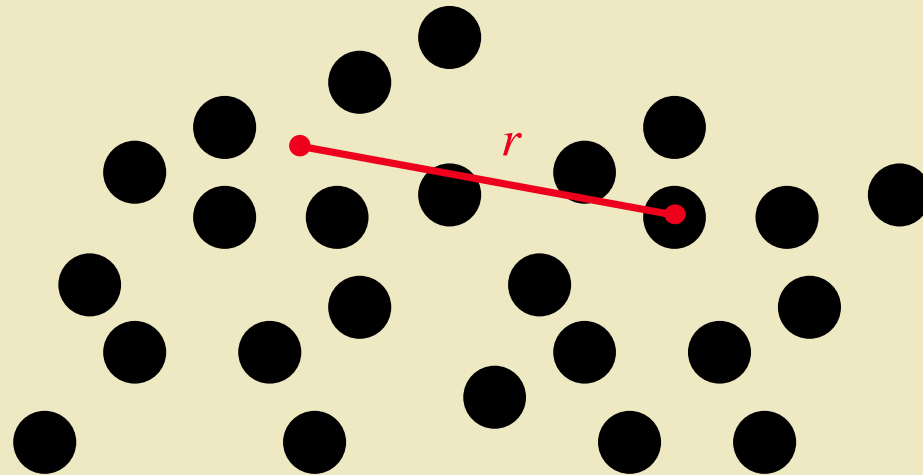
Decomposition series for the effective conductivity (physical constants, geometry, concentration):

$$\lambda_e = 1 + 2 \rho v + 2 \rho \sum_{p=2}^{\infty} A[\![p]\!] v^p$$

v denotes the concentration of inclusions,

$\rho = \dfrac{\lambda_1 - \lambda_0}{\lambda_1 + \lambda_0}$ contrast parameter.

$$A[\![2]\!] = \frac{\rho}{\pi} \frac{1}{n^2} \sum_{k_0, k_1}^{n} E_2 (a_{k_0} - a_{k_1}),$$

$E_p (z)$ stands for the Eisenstein
  function of order p (special function)

$$A[\![3]\!] = \frac{\rho^2}{\pi^2 n^3} \sum_{k_0, k_1, k_2}^{n} E_2 (a_{k_0} - a_{k_1}) \overline{E_2 (a_{k_1} - a_{k_2})}$$

$$A[\![4]\!] = \frac{1}{\pi^3 \, n^4} \left(-2 \, \rho^2 \sum_{k_0, k_1, k_2}^{n} E_3 \, (a_{k_0} - a_{k_1}) \, \overline{E_3 \, (a_{k_1} - a_{k_2})} \right.$$

$$\left. + \rho^3 \sum_{k_0, k_1, k_2, k_3}^{n} E_2 \, (a_{k_0} - a_{k_1}) \, \overline{E_2 \, (a_{k_1} - a_{k_2})} \, E_2 \, (a_{k_2} - a_{k_3}) \right)$$

$$A[\![5]\!] = \frac{1}{\pi^4} \left(6 \, \rho^2 \, e_{4,4} - 2 \, \rho^3 \, (e_{3,3,2} + e_{2,3,3}) + \rho^4 \, e_{2,2,2,2} \right)$$

$$A[\![6]\!] = \frac{1}{\pi^5} \left(-24 \, \rho^2 \, e_{5,5} + 6 \, \rho^3 \, (e_{4,4,2} + e_{3,4,3} + e_{2,4,4}) - \right.$$

$$\left. 2 \, \rho^4 \, (e_{3,3,2,2} + e_{2,3,3,2} + e_{2,2,3,3}) + \rho^5 \, e_{2,2,2,2,2} \right)$$

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A[[7]] =
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$$\frac{1}{\pi^6} \left(120\,\rho^2\,e_{6,6} - 24\,\rho^3\,(e_{2,5,5} + e_{3,5,4} + e_{4,5,3} + e_{5,5,2}) + 6\,\rho^4\right.$$

$$(e_{2,2,4,4} + e_{2,3,4,3} + e_{3,3,3,3} + e_{2,4,4,2} + e_{3,4,3,2} + e_{4,4,2,2}) -$$

$$24\,\rho^5\,(e_{2,2,2,3,3} + e_{2,2,3,3,2} + e_{2,3,3,2,2} + e_{3,3,2,2,2}) +$$

$$\left.\rho^6\,e_{2,2,2,2,2,2}\right)$$

Basic sums (include only locations of inclusions):

$$e_{m_1 \dots m_q} :=$$

$$N^{-\left[1 + \frac{1}{2}(m_1 + \dots + m_q)\right]} \sum_{k_0\,k_1\dots\,k_q} E_{m_1}(a_{k_0} - a_{k_1})\,\overline{E_{m_2}(a_{k_1} - a_{k_2})} \dots C^{q+1}\,E_{m_q}(a_{k_{q-1}} - a_{k_q})$$

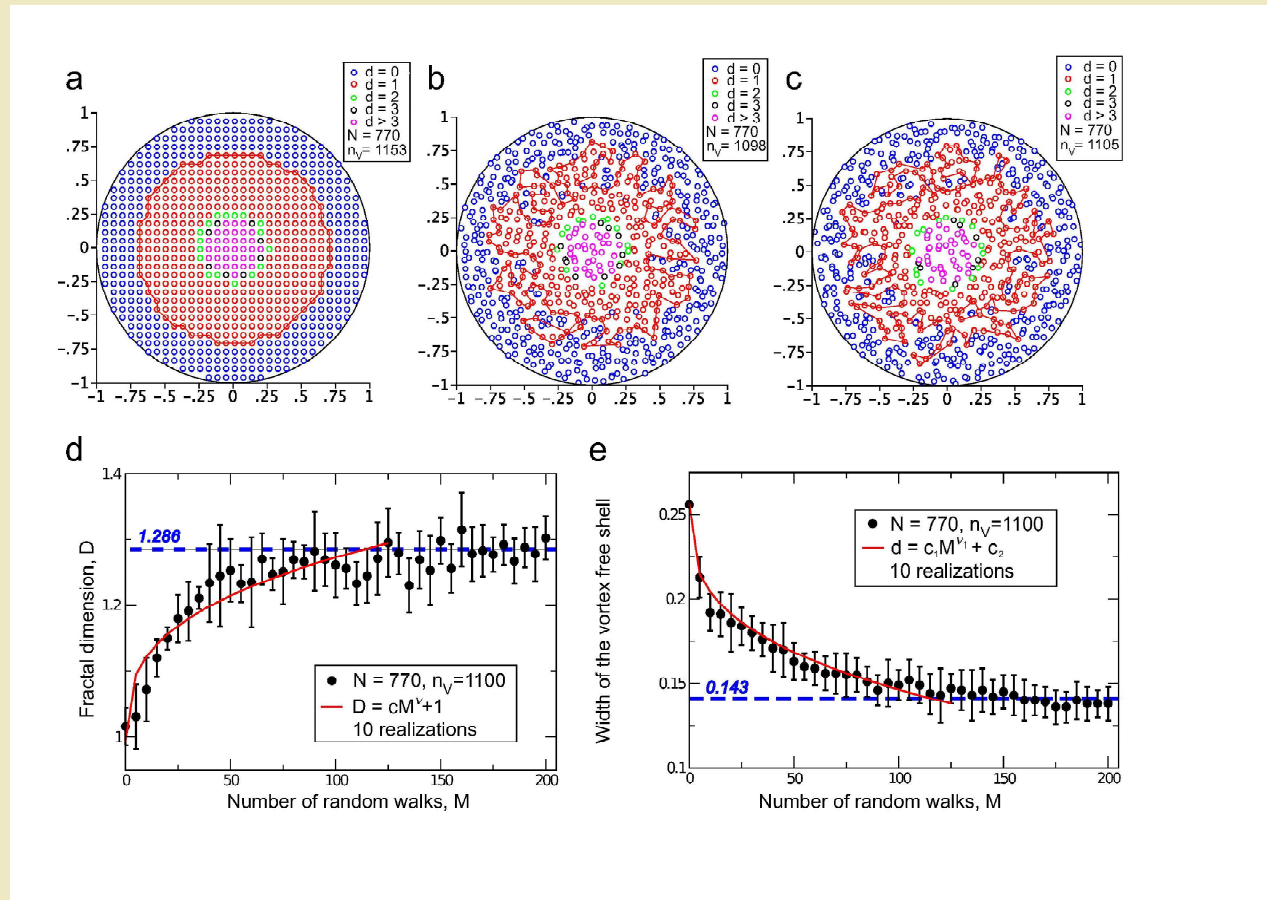multidimensional discrete chain convolutions
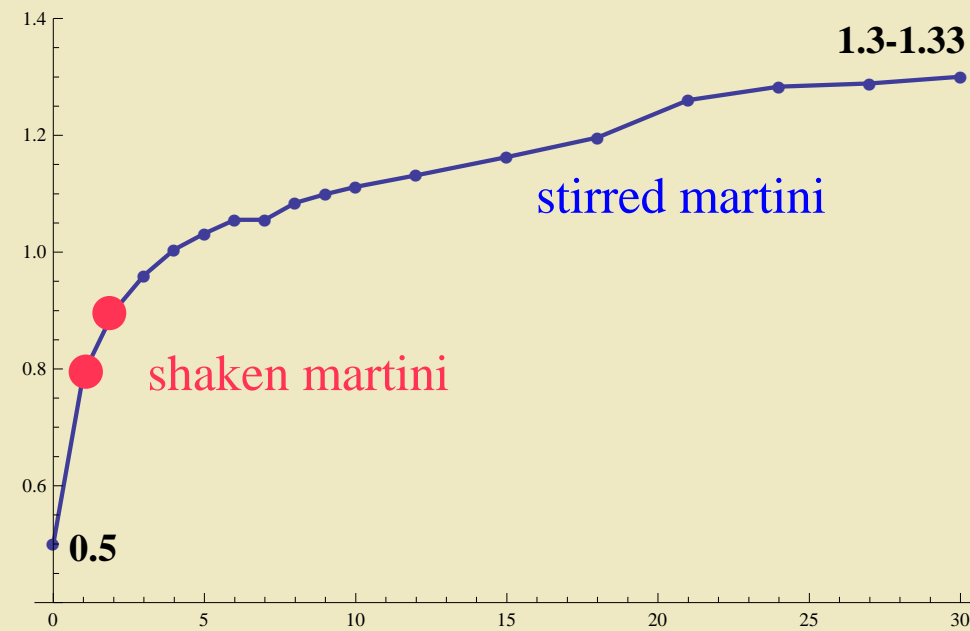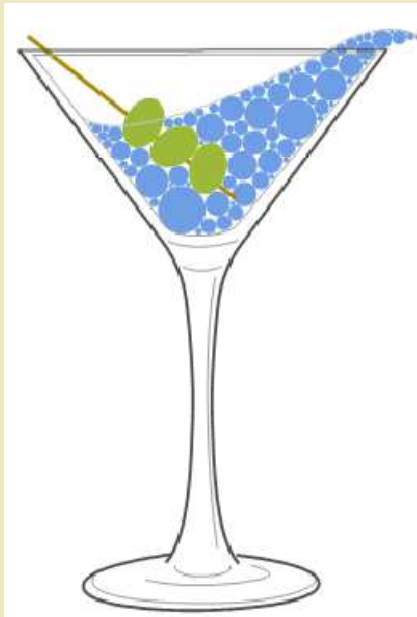
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Example (ρ = 1, ν concentration) :
λ[ν] = 1 + 2 ν + 2 ν² + 5.00392 ν³ + 6.3495 ν⁴ + 0.0000186711 ν⁹
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Fractal character of the level lines

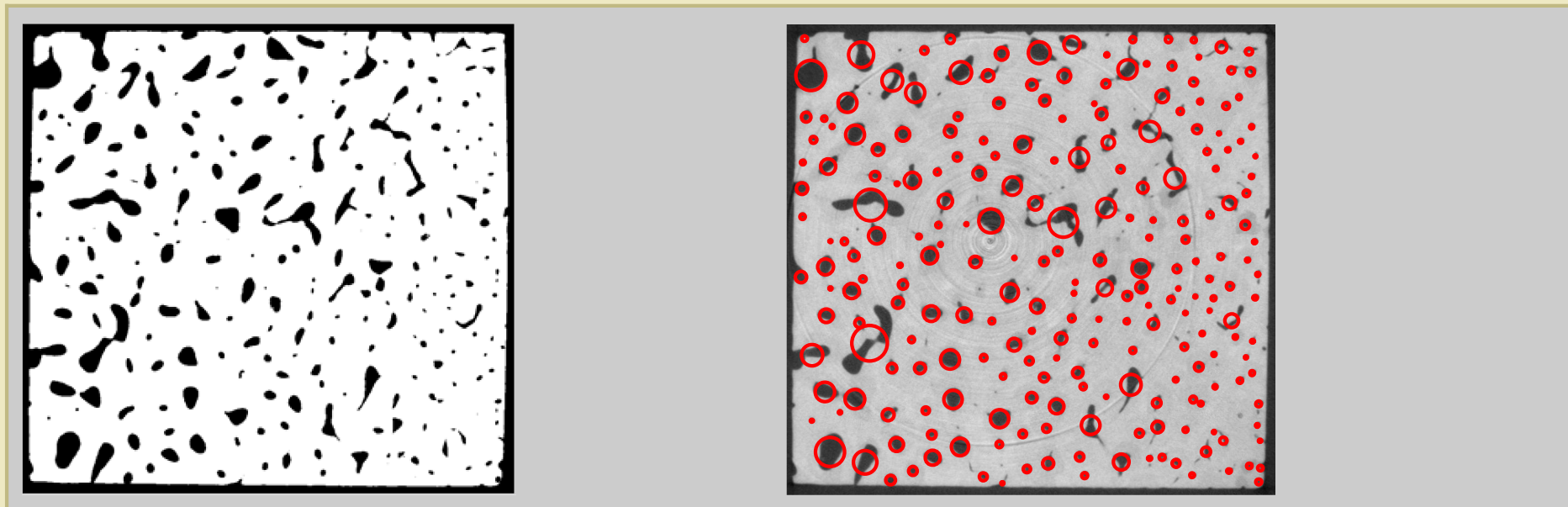S.D. Ryan, V. Mityushev, V. Vinokur, L. Berlyand, Scientific Reports, Nature Publ. (2015)

Critical power from regular to random

$$\lambda \simeq \frac{c}{\delta^s} \ , \ \delta \longrightarrow 0$$

Femoral neck; bone

■ Basic sums 1, polydispercity

$e_2 = 2.928 + 0.295 \, i$ has to be compared with $\pi \approx 3.14159$

	e_{22}	e_{33}	e_{2222}	e_{44}
theory	10.060	−0.408319	103.9329	1.0939

	e_{22}	e_{33}	e_{2222}	e_{44}
data 1	16.496	−17.93679	461.2028	68.458

- **Basic sums 2 with polydispercity (due to P. Kurtyka & N. Ryłko, AlSi$_9$ - 10% SiC)**

e_2 = 1.809 – 0.498 i

☐	e_{22}	e_{33}	e_{2222}	e_{44}
theory	10.060	–0.408319	103.9329	1.0939

| **data 2** | 34.101 | –82.10374 | 2779.583 | 1169.19 |

■ **Basic sums 2 with monodispercity**

$$e_2 = 3.012 + 1.2579\,i$$

□	e_{22}	e_{33}	e_{2222}	e_{44}
theory	10.060	−0.408319	103.9329	1.0939

data 2	38.4438	−245.39	178.0058	1773.0019

Basic sums 3
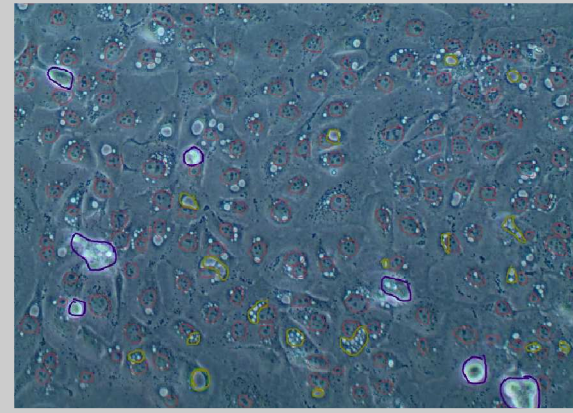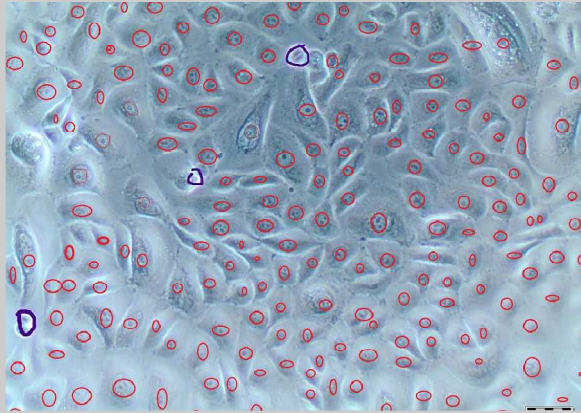
Healthy and ill human cells

healthy	e_2	e_{22}	e_{2222}	e_{33}	e_{44}
	$3.06 + 0.17\,i$	21.39	$83.7 + 18.4\,i$	-61.1	466

ill	e_2	e_{22}	e_{2222}	e_{33}	e_{44}
	$4.80 + 1.48\,i$	245	$3425 + 3245\,i$	-6355	$338\,814$

(not published results)

Thank you for your attention