Network models of biological structures

cn2017, June 20-23, 2017
Łądek Zdrój, Poland

Vladimir Mityushev

Department of Computer Sciences,
Pedagogical University,
Krakow, Poland
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)
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 randomly distributed objects.
Example: from one bacterium to self-organization and collective behavior of bacteria

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?
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,
\( \rho = \frac{\lambda_1 - \lambda_0}{\lambda_1 + \lambda_0} \) 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)

\[ A[3] = \frac{\rho^2}{\pi^2 n^3} \sum_{k_0, k_1, k_2}^n E_2 (a_{k_0} - a_{k_1}) E_2 (a_{k_1} - a_{k_2}) \]
\[ A[4] = \frac{1}{\pi^3 n^4} \left( -2 \rho^2 \sum_{k_0, k_1, k_2} \mathbf{E}_3 (a_{k_0} - a_{k_1}) \mathbf{E}_3 (a_{k_1} - a_{k_2}) \right) \\
+ \rho^3 \sum_{k_0, k_1, k_2} \mathbf{E}_2 (a_{k_0} - a_{k_1}) \mathbf{E}_2 (a_{k_1} - a_{k_2}) \mathbf{E}_2 (a_{k_2} - a_{k_3}) \right) \]

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

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

Basic sums (include only locations of inclusions):
\[
e_{m_1...m_q} := \\
N^\left[ \frac{1}{2} (m_1+...+m_q) \right] \sum_{k_0,k_1...k_q} E_{m_1}(a_{k_0} - a_{k_1}) \overline{E_{m_2}(a_{k_1} - a_{k_2})} ... C^{q+1} E_{m_q}(a_{k_{q-1}} - a_{k_q}) \]

multi-dimensional discrete chain convolutions

Example (\( \rho = 1, \ \nu \) concentration):
\[ \lambda[\nu] = 1 + 2 \nu + 2 \nu^2 + 5.00392 \nu^3 + 6.3495 \nu^4 + 0.0000186711 \nu^9 \]
Fractal character of the level lines

Critical power from regular to random

\[ \lambda \approx \frac{c}{\delta^s}, \quad \delta \rightarrow 0 \]
Femoral neck; bone
## Basic sums 1, polydisperscity

\[ e_2 = 2.928 + 0.295 \text{ has to be compared with } \pi \approx 3.14159 \]

<table>
<thead>
<tr>
<th></th>
<th>(e_{22})</th>
<th>(e_{33})</th>
<th>(e_{2222})</th>
<th>(e_{44})</th>
</tr>
</thead>
<tbody>
<tr>
<td>theory</td>
<td>10.060</td>
<td>-0.408319</td>
<td>103.9329</td>
<td>1.0939</td>
</tr>
<tr>
<td>data 1</td>
<td>16.496</td>
<td>-17.93679</td>
<td>461.2028</td>
<td>68.458</td>
</tr>
</tbody>
</table>
Basic sums 2 with polydispersity (due to P. Kurtyka & N. Ryłko, AlSi₉ - 10% SiC)

\[ e_{2} = 1.809 - 0.498 \hat{e} \]

<table>
<thead>
<tr>
<th></th>
<th>( e_{22} )</th>
<th>( e_{33} )</th>
<th>( e_{2222} )</th>
<th>( e_{44} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>theory</td>
<td>10.060</td>
<td>-0.408319</td>
<td>103.9329</td>
<td>1.0939</td>
</tr>
<tr>
<td>data 2</td>
<td>34.101</td>
<td>-82.10374</td>
<td>2779.583</td>
<td>1169.19</td>
</tr>
</tbody>
</table>
Basic sums 2 with monodisperscity

\[ e_2 = 3.012 + 1.2579 \bar{i} \]

<table>
<thead>
<tr>
<th></th>
<th>(e_{22})</th>
<th>(e_{33})</th>
<th>(e_{2222})</th>
<th>(e_{44})</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>theory</strong></td>
<td>10.060</td>
<td>-0.408319</td>
<td>103.9329</td>
<td>1.0939</td>
</tr>
<tr>
<td><strong>data 2</strong></td>
<td>38.4438</td>
<td>-245.39</td>
<td>178.0058</td>
<td>1773.0019</td>
</tr>
</tbody>
</table>
## Basic sums 3

Healthy and ill human cells

<table>
<thead>
<tr>
<th></th>
<th>$e_2$</th>
<th>$e_{22}$</th>
<th>$e_{2222}$</th>
<th>$e_{33}$</th>
<th>$e_{44}$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>healthy</strong></td>
<td>$3.06 + 0.17i$</td>
<td>$21.39$</td>
<td>$83.7 + 18.4i$</td>
<td>$-61.1$</td>
<td>$466$</td>
</tr>
<tr>
<td><strong>ill</strong></td>
<td>$4.80 + 1.48i$</td>
<td>$245$</td>
<td>$3425 + 3245i$</td>
<td>$-6355$</td>
<td>$338814$</td>
</tr>
</tbody>
</table>

(not published results)
Thank you for your attention