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## APPLICATION OF AI AND MACHINE LEARNING TO THE THEORY OF COMPOSITE MATERIALS

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The homogenization for classifying composites and determining their effective properties is an important optimal design problem of material sciences studied by mathematical modeling. The application of artificial intelligence (AI) and machine learning (ML) in the theory of composite materials is discussed. One of the main problems is the choice of characteristic ML features to describe multi-scale dispersed random composites and to predict their macroscopic properties. The complexity drastically increases when confronted with tasks such as estimating the effective properties of random composites, exploring optimal design scenarios with variable properties of components, or determining the optimal location and shape of inclusions since the myriad use of numerical computations proves challenging due to constraints in time and memory. In such instances, analytical, exact, or approximate formulas with the optimized parameters in symbolic form are preferred because powerful calculus methods can be applied to select the optimal parameters. The present paper is devoted to adequately choosing the parameters called structural sums, and corresponding analytical formulas. Such a formula is often asymptotic, and its correctly determined asymptotic precision shows its application area. We consider the question of the RVE size equivalent to the number of inclusions  $N$  per periodicity cell. It can be investigated numerically by solving a periodicity problem with  $N$  increasing up to stable effective constants not depending on  $N$ . Though one can find works in literature following these lines, they concern special distributions of inclusions with the numerical results performed for small  $N$  and for a small number of statistically investigated samples. A comprehensive study of 2D two-phase composites with equal circular inclusions is developed. It is demonstrated that using the concentration of inclusions and a contrast parameter is insufficient to properly study dispersed composites. The method of structural sums in combination with ML to improve model accuracy is applied. Based on the study, a new approach is suggested for selecting optimal parameters to analyze and classify two-dimensional dispersed composite structures. The included content fits *2020 Mathematics Subject Classification: 74Q15, 74-10*.

**Keywords:** artificial intelligence, machine learning, composite material, multi-scale problem, microstructure, homogenization, structural sum

### INTRODUCTION

Composites consist of two or more constituent materials with distinct physical properties used in engineering. The theory of composites is an important part of material sciences concerning hetero-

geneous media as well as mathematical and computational methods to determine their macroscopic properties. The mathematical theory of composites, the homogenization theory [1, 2, 3], is based on the measure theory and partial differential equations with highly oscillating coefficients. The computational methods involve predicting and understanding their behavior through advanced computer simulations. Artificial intelligence (AI) and machine learning (ML) have recently emerged as powerful tools. AI and ML enable the development of predictive models based on extensive datasets generated from experiments and simulations. The main task of these models is to accurately predict the elastic, thermal, and electrical properties of composites.

The description of the microstructure of composites is the first crucial task. Image processing algorithms [4, 5] analyze micrographs from microscopy and tomography, identifying the physical properties of structures and geometric features. Convolution neural networks are used to analyze microstructural images, classify different phases, and detect their locations in addition to various defects, such as fractures or holes.

The second crucial step is the constructive homogenization of the processed images to classify the considered composites and estimate their effective properties. In previous works, the second step was reduced to a statistical description of phases and direct computation by standard packages based on the finite element method (FEM). The opinion that a computer can calculate the effective constants of any composite is widely known in the engineering community. The numerical computation of effective constants becomes a virtually impossible task for dispersed random composites with many inclusions ( $\geq 1000$ ). Simple empirical equations were proposed to determine the effective constants in engineering. Many of them are oversimplified to be applied to composites. Using AI and ML without preliminary analysis of the used parameters significantly complicates the study and also leads to oversimplified models.

In the present paper, we discuss the constructive implementation of the theory of composites following Albert Einstein, who said: "Everything should be made as simple as possible, but not simpler." We analyze the methodological trends suggested by AI/ChatGPT and propose the choice of an optimal set of key parameters. We demonstrate that the method of structural sums [6, 7] in combination with ML can serve as a practical study method in the theory of composites, particularly for the classification of two-dimensional dispersed random structures.

### **Straightforward application of various methods to the analysis of composites**

The constructive homogenization of processed images allows classification of the considered composites and estimation of their effective properties. For definiteness, we consider the conductivity of two-dimensional (2D) two-phase dispersed composites modeling the flux in fiber reinforced composites.

The description of the phases goes by the following lines. Let the phases in a dispersed composite be determined in a representative volume element, and their properties be known. For instance, a set of  $N$  phases can be described by pairs  $\{\lambda_j, f_j\}$  ( $j = 1, 2, \dots, N$ ) where  $\lambda_j$  denotes the conductivity of  $j$ th phases and  $f_j$  its volume fraction in the considered composites. Pairs  $\{(\mu_j, \nu_j), f_j\}$  can be considered for elasticity problems, where  $\mu_j$  and  $\nu_j$  stand for the shear modulus and Poisson's ratio, respectively. Engineers usually add to the above parameters the number of particles per representative volume element (RVE), describe their shapes, and make other straightforward observations. The empirical analysis may be extended to an advanced description of geometry [8].

The effective constants are determined by the different mean values of  $\{\lambda_j, f_j\}$ . Following the lines of [9], we now ask AI (ChatGPT) and refer to Wikipedia with the question, how to determine ef-

fective conductivity  $\lambda_e$  with the selected information  $\{\lambda_j, f_j\}$  ( $j = 1, 2, \dots, N$ ). We also ask for the computational scheme for random composites from Wikipedia [https://en.wikipedia.org/wiki/Representative/\\_elementary/\\_volume](https://en.wikipedia.org/wiki/Representative/_elementary/_volume). Wikipedia presents a real image of the two-phase macroscopically isotropic dispersed composites shown on the left side of Figure 1. This picture displays a section perpendicular to a fibrous unidirectional composite.

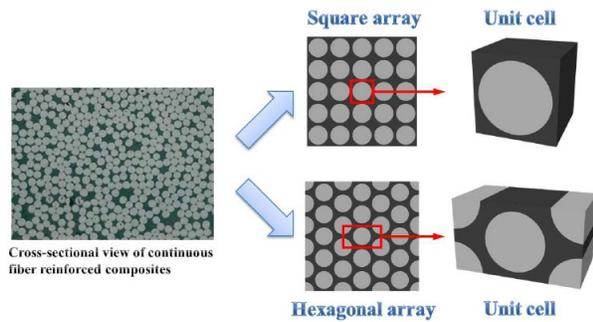


Fig. 1. Methodologically wrong scheme of RVE from Wikipedia [https://en.wikipedia.org/wiki/Representative/\\_elementary/\\_volume](https://en.wikipedia.org/wiki/Representative/_elementary/_volume). Random (left) and regular (right) composites in Figure 1 can have significantly different macroscopic properties in the case of percolation

ChatGPT gives information on the effective conductivity of dispersed 2D composites, as shown below in cursive font.

• **Parallel model (Reuss, 1929):**

$$\frac{1}{\lambda_e} = \frac{f}{\lambda_1} + \frac{1-f}{\lambda} := \left\langle \frac{1}{\lambda(\mathbf{x})} \right\rangle. \quad (1)$$

• **Series model (rule of mixtures by Voigt, 1889):**

$$\lambda_e = \frac{1}{|Q|} \int_Q \lambda(\mathbf{x}) \, d\mathbf{x} = f\lambda_1 + (1-f)\lambda := \langle \lambda(\mathbf{x}) \rangle. \quad (2)$$

*Keep in mind that these models make certain assumptions and may not apply to all fiber reinforced composites. The actual behavior of a specific composite may depend on factors such as fiber orientation, thermal contact resistance, and other microstructural details.*

• **Bruggeman equation:**

$$f \frac{\lambda_1 - \lambda_e}{\lambda_1 + \lambda_e} + (1-f) \frac{\lambda - \lambda_e}{\lambda + \lambda_e} = 0. \quad (3)$$

• **Voigt-Reuss bounds:**

$$\left\langle \frac{1}{\lambda(\mathbf{x})} \right\rangle \leq \lambda_e \leq \langle \lambda(\mathbf{x}) \rangle. \quad (4)$$

• **Hashin-Shtrikman bounds:** *The effective conductivity of any 2D macroscopically isotropic two-phase composite satisfies the Hashin-Shtrikman bounds*

$$\lambda^- \leq \lambda_e \leq \lambda^+. \quad (5)$$

*If  $\lambda_1 > \lambda$ , the bounds are expressed as:*

$$\lambda^+ = \lambda_1 \left[ 1 + \frac{2(1-f)(\lambda - \lambda_1)}{f(\lambda - \lambda_1) + 2\lambda_1} \right], \quad (6)$$

$$\lambda^- = \lambda \left[ 1 + \frac{2f(\lambda_1 - \lambda)}{(1-f)(\lambda_1 - \lambda) + 2\lambda} \right]. \quad (7)$$

*If  $\lambda_1 < \lambda$ , the upper and lower bounds are swapped.*

*Additionally, other models and approaches, such as the Maxwell model or Mori-Tanaka method, can be used to estimate effective properties and may provide different insights depending on the specifics of the composite material and its structure.*

We now analyze the mined information using fundamental mathematical investigations [1, 2, 3, 6, 7] and make comments. Formulas (1)-(2) look sensible, but their careful study suggests that they are valid for layered composites, not dispersed media. One can note that (1)-(2) coincide with effective conductivity perpendicular and parallel to the fibers,  $\lambda_{\perp} = \left\langle \frac{1}{\lambda(\mathbf{x})} \right\rangle$  and  $\lambda_{\parallel} = \langle \lambda(\mathbf{x}) \rangle$ , and yield the Voigt-Reuss bounds (4). The note after (2) is correct.

Hashin-Shtrikman bounds (5)-(7) improve the Voigt-Reuss bounds and give the most valuable information for composites when the location of inclusions is not known. Using (5)-(7) makes it easy to check the validity of empirical models such as Bruggeman's approximation based on the correct opinion that anybody may sketch any curve between

the Hashin-Shtrikman bounds displayed in Figure 2. It does not matter which curve is taken in the case  $\frac{\lambda_1}{\lambda} = 5$ . Nevertheless, it does in the case  $\frac{\lambda_1}{\lambda} = 50$ .

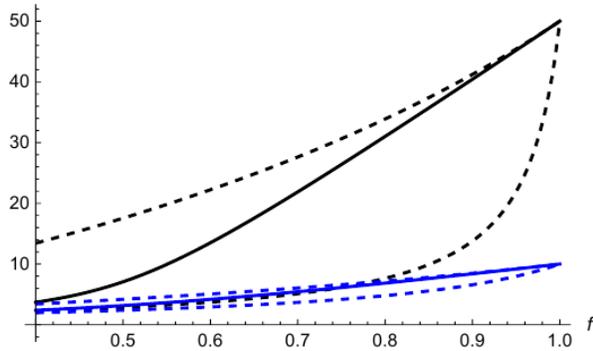


Fig. 2. Hashin-Shtrikman bounds (0.5)-(0.7) (dashed lines) and Bruggemann heuristic equation (0.3) (solid line) for:  $\lambda_1 = 50$ ,  $\lambda = 10$  (black) and  $\lambda_1 = 5$ ,  $\lambda = 1$  (blue)

It is worth noting that Bruggeman's approximation may be out of the higher-order bounds [10].

The paragraph after (7) contains the information which has to be analyzed as Bruggemann's approximation [12].

Figure 1 demonstrates the methodologically wrong scheme of the RVE when a regular array replaces a random composite. One can find exact analytical formulas for the effective conductivity of regular arrays in [6] and approximate analytical formulas for elastic problems in [7]. It turns out that the effective conductivity of the hexagonal array of disks attains a minimum if  $\lambda_1 > \lambda$ . Therefore, the scheme in Figure 1 leads to extreme values of  $\lambda_e$ , not adequately representing a class of random composites. This misleading scheme implies a numerical solution to the problems for the unit cells depicted in the third column of Figure 1. Moreover, the double periodicity cell for the hexagonal array is presented as a unit cell that doubles the discretization domain.

## Method of structural sums

Let the location of the inclusions in the left picture of Figure 1 be given. The numerical solution

to the considered problem for small fragments of the picture can be performed using standard engineering simulation software.

The complexity drastically increases when confronted with tasks such as estimating the effective properties of random composites, exploring optimal design scenarios with variable properties of components, or determining the optimal location and shape of inclusions since the myriad use of numerical computations proves challenging due to constraints in time and memory.

In such instances, analytical, exact, or approximate formulas with the optimized parameters in symbolic form are preferred because powerful calculus methods can be applied to select the optimal parameters. The present section is devoted to adequately choosing the parameters and corresponding analytical formulas. Such a formula is often asymptotic, and its correctly determined asymptotic precision shows its application area.

The question of the RVE size equivalent to the number of inclusions  $N$  per cell arises naturally. It can be investigated numerically by solving a periodicity problem with  $N$  increasing up to stable effective constants not depending on  $N$ . Though one can find works in literature following these lines, they concern special distributions of inclusions with the numerical results performed for small  $N$  and for a small number of statistically investigated samples.

In this case, asymptotic and analytical methods can be helpful. Consider 2D two-phase composites with equal circular inclusions of conductivity  $\lambda_1$  and matrix conductivity  $\lambda$ , represented by cell  $Q$  of the normalized unit area. Introduce the dimensionless contrast parameter

$$q = \frac{\lambda_1 - \lambda}{\lambda_1 + \lambda}, \quad (8)$$

Consider Eisenstein functions  $E_p(z)$  [11] expressed in terms of the Weierstrass elliptic functions

$$\begin{aligned} E_2(z) &= \wp(z) + S_2, \quad E_3(z) = \\ &= -\frac{1}{2}E'_2(z) = -\frac{1}{2}\wp'(z), \quad \dots, \end{aligned} \quad (9)$$

where lattice sum  $S_2 = \pi$  for unit square fundamental domain  $Q$  considered below for the plane torus, see Figure 3.

The structural sums can be introduced following [6]

$$e_2 = \frac{1}{N^2} \sum_{k_0, k_1=1}^N E_2(a_{k_0} - a_{k_1}),$$

$$e_{pp} = \frac{1}{N^{1+p}} \sum_{k_0, k_1, k_2=1}^N E_p(a_{k_0} - a_{k_1}) E_p(a_{k_1} - a_{k_2}) \quad (p = 2, 3), \quad (10)$$

$$e_{222} = \frac{1}{N^4} \sum_{k_0, k_1, k_2, k_3=1}^N E_2(a_{k_0} - a_{k_1}) E_2(a_{k_1} - a_{k_2}) E_2(a_{k_2} - a_{k_3}),$$

... ..,

where it is assumed for shortness that  $E_2(a_k - a_m) = S_2$  and  $E_3(a_k - a_m) = 0$ , if  $a_k = a_m$ .

The structural sum (0.10) is a discrete multiple convolution of the Eisenstein functions. A fast, almost linear algorithm in  $N$  for its computation was developed in [7].

Using complex structural sums, we form matrix structural sums

$$\mathbf{e}_{m_1, \dots, m_q} = \begin{pmatrix} \text{Re } e_{m_1, \dots, m_q} & -\text{Im } e_{m_1, \dots, m_q} \\ -\text{Im } e_{m_1, \dots, m_q} & \text{Re } e_{m_1, \dots, m_q}^* \end{pmatrix}, \quad (11)$$

where  $e_{m_1, \dots, m_q}^*$  has the same form (10) except at terms  $E_2(a_k - a_m)$ , which have to be replaced by the expressions  $2\pi - E_2(a_k - a_m)$ .

The effective conductivity tensor has the form

$$\frac{\lambda_{\perp}}{\lambda} = (1 + 2\varrho f) \mathbf{I} + \frac{2\varrho^2 f^2}{\pi} \mathbf{e}_2 + \frac{2\varrho^3 f^3}{\pi^2} \mathbf{e}_{22} + \frac{2\varrho^3 f^4}{\pi^3} (\varrho \mathbf{e}_{222} - 2\mathbf{e}_{33}) + O(f^5), \quad (12)$$

where  $\mathbf{I}$  is the identity matrix. The series (0.12) can be easily extended; see the high-order formulas in  $f$  in [6].

A series of relations was established in [13] for macroscopically isotropic composites. In particular,

$$e_2 = \pi, \quad e_{222} = 2\pi e_{22} - \pi^3. \quad (13)$$

Moreover, the following computationally effective formulas were derived in [13]

$$e_{22} = \frac{1}{N^3} \sum_{k=1}^N \left| \sum_{m=1}^N E_2(a_k - a_m) \right|^2, \quad e_{33} = -\frac{1}{N^4} \sum_{k=1}^N \left| \sum_{m=1}^N E_3(a_k - a_m) \right|^2. \quad (14)$$

Formulas (13) and (14) after substitution into (12) yield the following formula for the effective conductivity of macroscopically isotropic composites

$$\frac{\lambda_e}{\lambda} = 1 + 2\varrho f + 2\varrho^2 f^2 + \frac{2\varrho^3 f^3}{\pi^2} e_{22} + \frac{2\varrho^3 f^4}{\pi^2} ((2e_{22} - \pi^2)\varrho - 2\pi e_{33}) + O(f^5). \quad (15)$$

It is worth noting that  $e_{22} = \pi^2$  and  $e_{33} = 0$  for the hexagonal and square regular arrays. Hence, (15) becomes

$$\frac{\lambda_{hex}}{\lambda} = 1 + 2\varrho f + 2\varrho^2 f^2 + 2\varrho^3 f^3 + 2\varrho^4 f^4 + O(f^5). \quad (16)$$

More accurate formulas up to  $O(f^{27})$  can be found in [6].

## Computer simulations

We are interested in random composites. Let contrast parameter  $\varrho$ , the radius of inclusions, and concentration  $f$  be fixed. Consider a class of random composites  $\mathcal{K}(f)$ , whose centers form the uniform i.i.d. (independent and identically distributed) random variables. Class  $\mathcal{K}(0)$  is determined by the Poisson point process. Class  $\mathcal{K}(\frac{\pi}{\sqrt{12}})$  contains one element, the hexagonal array of touching disks. Structural sums  $e_{22}$  and  $e_{33}$  can be considered as random variables determined in a class  $\mathcal{K}(f)$ .

The feature vector of structural sums was studied by machine learning tools and data analysis

[14], where the classification method for composites with circular inclusions and composites with shapes formed by disks was developed. Structural sums  $e_{33}$  and  $e_{88}$  were selected for analysis after the conjecture that  $e_{88}$  is related to the heterogeneity of disks in a pattern and  $e_{33}$  the clustering of disks. An irregularity measure of a sample similar to entropy was proposed [14]

$$\mu_{Naw} = \log(1 - e_{33})(1 + e_{88}). \quad (17)$$

It should be noted that the regular hexagonal array of disks yields  $e_{33} = e_{88} = 0$ , hence,  $\mu_{Naw} = 0$ .

In the present section, we consider feature vector  $(e_{22}, e_{33})$  determining macroscopically isotropic composites in accordance with (15) up to  $O(f^5)$ . We also suggest a new formula for the irregularity measure, which includes concentration  $f$

$$\mu(f) = (1 + 2f) \log \frac{e_{22}}{\pi^2} + 2f \log(1 - e_{33}). \quad (18)$$

It was proved in [13] that  $e_{22} \geq \pi$  and  $e_{33} \leq 0$  for any non-overlapping location of disks. The expected value of feature vector  $(e_{22}, e_{33})$  depends on  $f$ , hence, on radius  $r$ .

Below, the computational experiments are performed for classes of composites  $\mathcal{K}_\alpha(f)$ , where  $0 \leq \alpha \leq 1$ . Class  $\mathcal{K}(f) \equiv \mathcal{K}_1(f)$  is defined at the beginning of this section. Here, the centers are simulated with a radius  $r$  corresponding to concentration  $f_0 = N\pi r^2$  and  $0 \leq f \leq f_0$ . Any two different centers of  $\mathcal{K}(f)$  satisfy inequality  $|a_k - a_m| \geq 2r$ . Class  $\mathcal{K}_\alpha(\alpha^2 f)$  is a similar class for which  $|a_k - a_m| \geq 2\alpha r$ . This class corresponds to Keller's concept of a "security" sphere (disk) [15, page 565]. It is convenient to consider classes with the same concentration, i.e. instead of  $\mathcal{K}_\alpha(\alpha^2 f)$  to consider the equivalent class  $\mathcal{K}_\alpha(f)$ , where  $\alpha = \sqrt{\frac{f}{f_0}}$ .

An example of  $N = 300$  points is presented in Figure 3. The coordinates of the points in Figure 3a are simulated by the sequence location of disks [16] in the unit square with  $r = 0.02$ , hence, with concentration  $f_0 = 0.3770$ . A location from class  $\mathcal{K}(0.3770)$  is presented in Figure 3a. The

coordinates of the points in Figures 3a and 3b coincide. Therefore, a location from class  $\mathcal{K}_{\frac{1}{2}}(0.0942)$  is presented in Figure 3b, where  $\frac{1}{4}f_0 = 0.0942$ . This means that the structural sums of the configurations in Figures 3a and 3b coincide, but the entropy (18) does not.

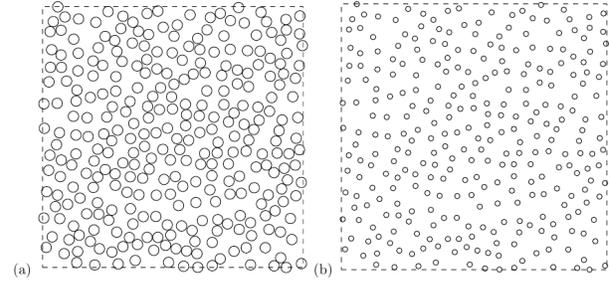


Fig. 3. Simulation of non-overlapping disks: a) class  $\mathcal{K}_1(0.3770)$  with concentration  $f_0 = 0.3770$ ; b) class  $\mathcal{K}_{\frac{1}{2}}(0.0942)$  with concentration  $\frac{1}{4}f_0 = 0.0942$ . Centers of disks coincide

Statistical data for  $(e_{22}, e_{33})$  are selected by the following procedure. The computational experiment is conducted to research the structural sums in composite materials using non-overlapping circles uniformly distributed in a square area. The main goal of the experiment is to calculate structural sums  $e_{22}$  and  $e_{33}$  for randomly generated circles and their further interpretation. Structural sums allow us to quantify the interactions between inclusions in a composite and are important for understanding such effective material properties as thermal conductivity.

For each experimental variant, a new set of circle centers is created, and for each set, structural sums  $e_{22}$  and  $e_{33}$  are calculated. The first step in the simulation is to generate non-overlapping circles inside a square. The circles are randomly placed, and each new circle should not overlap with the existing ones.

The Weierstrass (Eisenstein) elliptic functions are used to analyze the structure generated by circles, which are suitable for modeling periodic two-dimensional systems. Functions  $E_2$  and  $E_3$  are derived from the Weierstrass functions and are used in calculating structure sums  $e_{22}$  and  $e_{33}$ .

A point graph for 100 experiments shows the computed values of  $e_{22}$  in Figure 4. The number of experiments  $t$  is displayed on the  $x$ -axis and  $e_{22}$  on the  $y$ -axis. The graph shows values fluctuating between 11.5 and 13.0. The width of the red dashed line is equal to the double standard deviation of  $e_{22}$ .

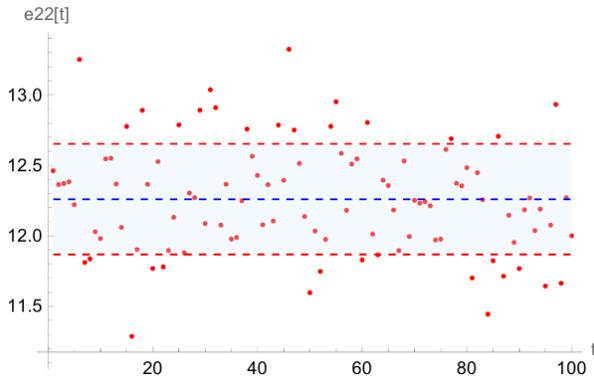


Fig.4. Values of  $e_{22}$  with mean value (dashed blue line) and standard deviation ranges (dashed red lines)

In Figure 5, the analogous point graph shows the computed values of  $e_{33}$  for 100 experiments, with the results ranging between  $-6.5$  and  $-5.0$  across the iterations.

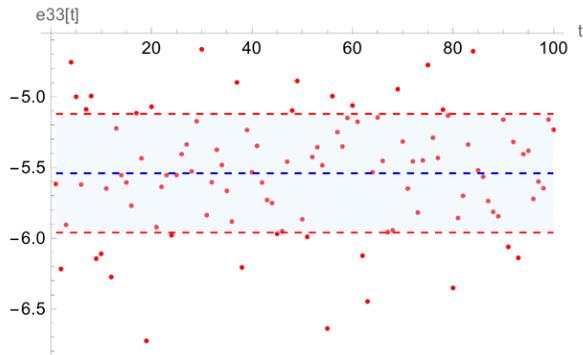


Fig. 5. Values of  $e_{33}$  with mean value (dashed blue line) and standard deviation ranges (dashed red lines)

The histograms of  $e_{22}$  and  $-e_{33}$  values in Figures 6 and 7, respectively, show the frequency of the occurrence of results across the experiments. This helps to understand the distribution of the structural sums.

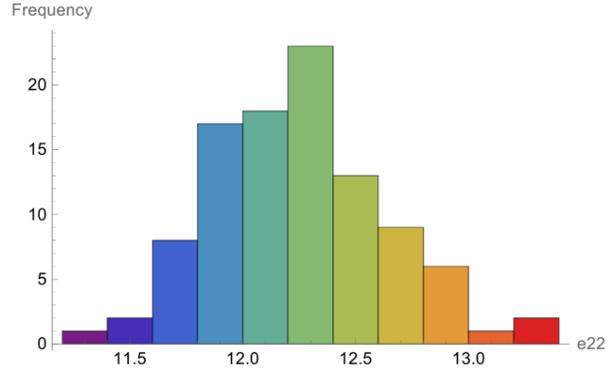


Fig. 6. Histogram of frequency of  $e_{22}$  values depending on number of experiments

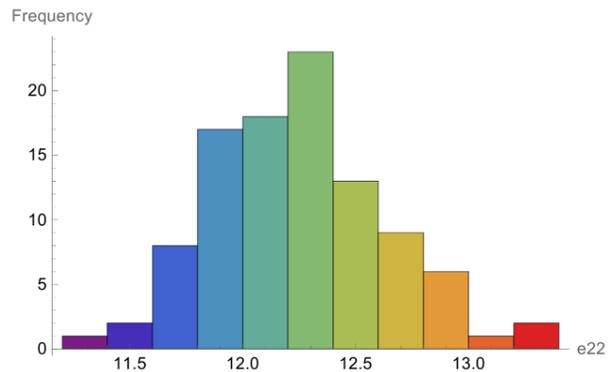


Fig. 7. Histogram of frequency of  $-e_{33}$  values depending on number of experiments

Figure 8 shows the relationship between the values of  $e_{22}$  and  $e_{33}$ . It can be considered a phase space set used in the ML of the considered class of simulated composite.

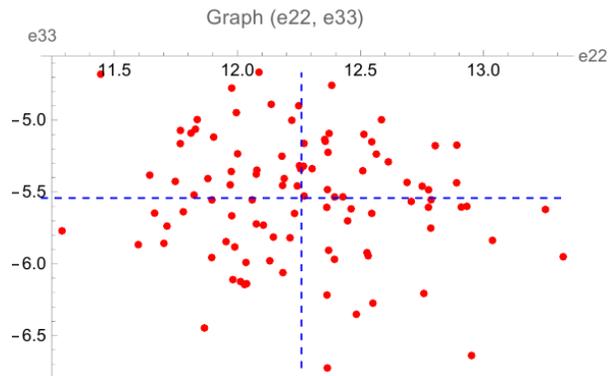


Fig. 8. Relationship between structural sums  $e_{22}$  and  $e_{33}$ . Points represent data for each experiment

The computed structural sums are used to analyze the effective properties of the considered composites. For instance, the sums are applied to estimate the effective conductivity of the composite,  $\lambda_e$ , based on a theoretical formula that includes both  $e_{22}$  and  $e_{33}$ . An analogous phase space was used in [14] to classify classes of composites by ML.

The entropy values (18) are calculated for the simulated data and shown in Figures 9 and 12. The results are displayed for  $f = 0.125664$ ; the entropy range takes values from 2.26389 to 2.8992.

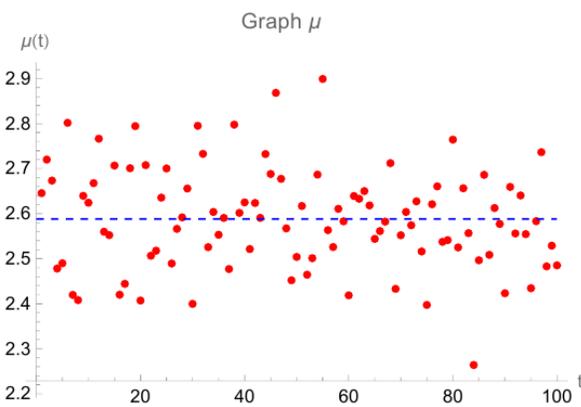


Fig. 9. Entropy values

Consider different classes of composites  $\mathcal{K}_\alpha(f)$  for fixed concentration  $f = 0.125664$ . We take the following number of centers:  $N = 100, 400, 900, 1600, 2500$ , and radii:  $r = 0.02, 0.01, 0.00667, 0.005, 0.004$ , respectively. In this case, the number of centers  $N$  and radii  $r$  of the circles are related by the ratio  $f = \pi r^2 N$  with fixed  $f = 0.125664$ . The ML phase set of all the points is displayed in Figure 10. The set of their mean values over every class is presented in Figure 11, together with the circles equal to the standard deviation of the points of every class.

The mean values of  $e_{22}$  and  $e_{33}$  were calculated for each experimental variant. These mean values served as the centers of the circles on the graph. For instance, if the mean value of  $e_{22}$  is 24.86 and the mean value of  $e_{33}$  is  $-54.5$ , the center of the circle will be located at the point  $(24.86, -54.5)$ .

The radius of each circle corresponded to the standard deviation of  $e_{22}$  and  $e_{33}$  for that particular dataset. The standard deviation shows how much the values fluctuate around the mean. Thus, a larger radius indicates more variability in the structural sums for that set of circles.

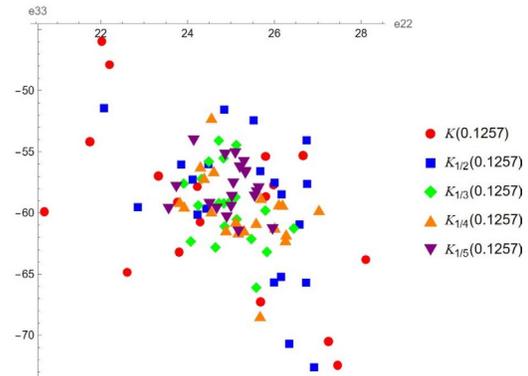


Fig. 10. ML phase space  $e_{22}$  and  $e_{33}$

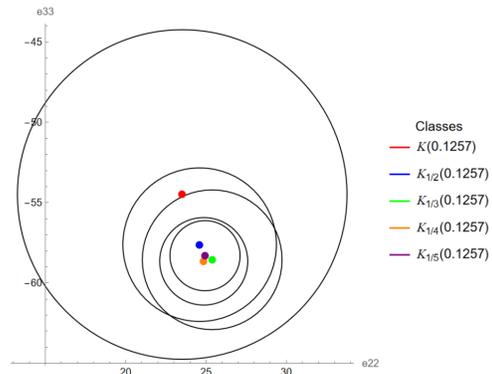


Fig. 11. Centers of circles correspond to mean values of  $e_{22}$  and  $e_{33}$ , while radii represent standard deviations

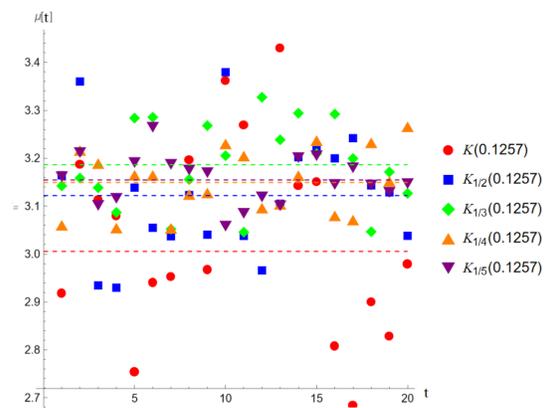


Fig. 12. Entropy (18) calculated for all simulated points

## CONCLUSIONS

These graphs help to quickly identify patterns or inconsistencies across different experimental configurations. If several circles are closely clustered with small radii, it indicates a more consistent and stable result. On the other hand, if there are large variations in the radii, it shows higher uncertainty or variation in the structural sums for that set of experiments. The degree of deviation can be considered an ML feature in the classification of composites.

Finally, the entropy values ( $\mu(f)$ ) are calculated based on the structure sums, which measure the disorder in the system. These entropy values are calculated for each experiment.

In the present paper, we consider the existing models suggested by AI and demonstrate that its recommendations should be carefully analyzed. Numerical calculation methods such as the FEM are not suitable for analyzing the effective conductivity of dispersed random composites due to their inherent limitations and impracticality. Before straightforward computations, we propose to use the constructive analytical theory of homogenization to select the optimal parameters: the structural sums besides the concentration and the contrast parameter. Such a choice essentially reduces the computations and suggests a new ML phase space used for the classification of two-dimensional composites.

## Author contributions

V.V. Mityushev served as the principal investigator and supervised the research process.

K.B. Nurtazina collected and analyzed the data, and led the manuscript preparation.

N.Zh. Nauryzbayev conducted computational experiments in Mathematica and assisted in data analysis.

All the authors participated in the revision of the manuscript and approved the final submission.

## Conflict of Interest

The authors declare that there is no conflict of interest.

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