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DEVELOPMENT OF AN ALGORITHM AND SOFTWARE FOR MODELING THE STRUCTURE AND MECHANICAL BEHAVIOR OF AEROGELS

Aerogels, known for their ultra-low density and exceptional physical properties such as high porosity, low thermal conductivity, and large specific surface area, represent a promising class of materials for a wide range of technological applications. These include insulation systems, catalyst supports, acoustic dampening, and even aerospace engineering. Despite their advantages, the complex and highly porous internal structure of aerogels poses significant challenges when it comes to accurately predicting their mechanical behavior under different loading conditions. Therefore, the development of computational models that realistically capture the microstructure of aerogels is a critical step in optimizing their performance and extending their practical use. This paper presents a comprehensive approach to modeling the structure and mechanical response of silica-based aerogels. At the heart of the modeling process lies the Diffusion-Limited Cluster-Cluster Aggregation (DLCA) algorithm, which is employed to generate computational representations of aerogel structures that closely mimic their real-world microarchitecture. The algorithm simulates the formation of aerogels by modeling the random motion and aggregation of primary particles into larger clusters, eventually forming a fractal-like porous network characteristic of aerogels. A dedicated software tool was developed to implement the DLCA algorithm and generate digital models of aerogel structures. To enable mechanical analysis, the output of this modeling process is converted into a finite element mesh using APDL (ANSYS Parametric Design Language) scripts. These scripts automate the creation of finite element models, which are then imported into the ANSYS simulation environment. Within ANSYS, the mechanical behavior of the generated structures is analyzed by applying simple loading conditions to assess displacements and stress distributions. The results of these test simulations provide valuable insights into how the internal geometry of aerogels influences their overall mechanical performance. This methodology not only aids in understanding the structure–property relationships in aerogels but also supports the design of improved materials tailored to specific engineering needs.

Keywords: aerogels, DLCA, computer modeling, software development.

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РОЗРОБКА АЛГОРИТМУ ТА ПРОГРАМНОГО ЗАБЕЗПЕЧЕННЯ ДЛЯ МОДЕЛЮВАННЯ СТРУКТУРИ ТА МЕХАНІЧНОЇ ПОВЕДІНКИ АЕРОГЕЛІВ

Аерогелі — це матеріали з надзвичайно низькою густиною та унікальними фізичними властивостями, такими як висока пористість, низька теплопровідність і велика питома площа поверхні. Вони є перспективними для широкого спектра технологічних застосувань, зокрема в теплоізоляції, носіях каталізаторів, поглиначах звуку та навіть в аерокосмічній галузі. Однак складна та високопориста внутрішня структура аерогелів створює серйозні труднощі при моделюванні їх механічної поведінки за різних навантажень. Тому розробка обчислювальних моделей, що достовірно відображають мікроструктуру аерогелів, є ключовим етапом для оптимізації їх властивостей і розширення можливостей практичного застосування. У цій роботі представлено комплексний підхід до моделювання структури та механічної поведінки аерогелів на основі діоксиду кремнію. Основою моделювання є алгоритм кластер-кластерної агрегації з дифузійним обмеженням (DLCA), за допомогою якого створюються обчислювальні представлення аерогелевих структур, що імітують їх реальну мікроархітектуру. Алгоритм моделює утворення аерогелів через випадковий рух і агрегацію первинних частинок у більші кластери, що формують фрактальноподібну пористу мережу — характерну ознаку аерогелів. Для реалізації алгоритму DLCA було розроблено спеціальне програмне забезпечення, яке генерує цифрові моделі структур аерогелів. З метою проведення механічного аналізу отримані структури перетворюються на скінченноелементну сітку за допомогою скриптів на мові APDL (ANSYS Parametric Design Language). Ці скрипти автоматизують створення моделей для імпорту в середовище моделювання ANSYS. У ANSYS проводиться аналіз механічної поведінки моделей шляхом прикладення простих навантажень для оцінки переміщень і розподілу напружень. Результати симуляцій дозволяють краще зрозуміти, як внутрішня геометрія аерогелів впливає на їх загальні механічні характеристики. Запропонована методика не лише поглиблює уявлення про взаємозв'язок між структурою та властивостями аерогелів, а й сприяє розробці вдосконалених матеріалів, оптимізованих під конкретні інженерні задачі.

Ключові слова: аерогелі, DLCA, комп'ютерне моделювання, розробка програмного забезпечення.

1. Introduction. Aerogels, particularly silica aerogels, exhibit exceptional properties, making them attractive for applications such as thermal insulation, space dust collection, and drug delivery. Investigating their mechanical properties is a critical research area, utilizing experimental, numerical, and AI-driven approaches.

Experimental studies examine key parameters like density, porosity, and microstructure, which significantly influence mechanical behavior. Techniques such as Small-Angle X-ray Scattering (SAXS) and Small-Angle Neutron Scattering (SANS) provide insights into the fractal nature of aerogels and their mass distribution [1].

The elastic modulus of aerogels often follows a power-law relationship with relative density, with exponents ranging from 2 to 4 depending on microstructural characteristics [2]. High porosity and low-density render aerogels brittle, with mechanical behavior heavily influenced by density [2].

Numerical modeling enables a deeper investigation of mechanical properties, employing molecular dynamics simulations, aggregation models, and multiscale techniques [1-4]. DLCA and Reaction-Limited Cluster Aggregation (RLCA) models simulate particle clustering processes, aiding in replicating experimental scattering curves and exploring mechanical properties [1-4].

Recent advances in AI-driven methods, particularly deep learning, facilitate material behavior prediction, microstructure optimization, and the discovery of new materials with unique properties [5,8-10]. Reinforcement learning methods enable autonomous material exploration, paving the way for rapid aerogel characterization and synthesis optimization [5-6, 8-9].

A combination of DLCA and the Finite Element Method (FEM) effectively evaluates the mechanical properties of aerogels [1, 5]. The DLCA method simulates

particle aggregation due to Brownian motion, forming clusters that represent aerogel networks. Hasmy et al. demonstrated that DLCA-generated structures closely match silica aerogel scattering data, making it a suitable modeling approach [1, 5, 10].

Following DLCA modeling, FEM is employed to analyze mechanical properties. A Representative Volume Element (RVE) based on DLCA-generated structures is created, considering periodic boundary conditions. In this model, particles serve as nodes, and the bonds between them as beams, capturing bending, torsion, and stretching deformations. The mechanical behavior of silica aerogels is analyzed through RVE compression simulations.

Historical research on sol-gel chemistry and fractal structures provided a theoretical foundation for modeling aerogels [11]. Recent micromechanical experiments using atomic force microscopy (AFM) have demonstrated localized stress responses in silica aerogels, reinforcing computational predictions [12]. At the same time, innovations in AI-based modeling such as AlphaFold illustrate the transformative impact of data-driven approaches on structural science [13]. Earlier studies on the production and properties of aerogels also remain relevant for understanding processing–structure relationships [14]. Moreover, molecular dynamics simulations have successfully captured the mechanical behavior of nanoporous aerogels, consistent with the results of this study [15].

2. Problem statement

- To develop computer models of aerogel structures, the following tasks must be completed:
- Develop algorithms for aerogel structure formation based on the DLCA algorithm.
- Implement software for executing the DLCA algorithm and generating corresponding structures.
- Develop APDL scripts to construct finite element models in ANSYS.
- Perform test calculations of displacements and stresses under simple loading conditions.

3. Description of the algorithm. The DLCA algorithm models aerogel structure formation by simulating silica nanoparticle aggregation through diffusion and adhesion dynamics. The process begins by defining a periodic simulation box containing randomly placed "walkers" and "seeds." Walkers follow a random-walk trajectory until reaching a critical adhesion distance, at which point they bond to a seed or another walker, forming clusters. The modeling process takes into account their random movement, diffusion, and adhesion. The method is based on selecting a representative volume to obtain a structure that matches experimental results.

The MATLAB-based modeling process allows customization of parameters such as particle radius, critical distance, seed and walker count, step size, adhesion probability, and movement type. To ensure periodicity, connections near box boundaries are adjusted through projection rules.

At the beginning of the modeling, it is necessary to set the boundary conditions in a periodic box, where random "walkers" and "seeds" are initialized. They can be placed randomly or in an orderly manner. In this specific example, the "walkers" are placed randomly and move according to the theory of random walks, with steps defined for both "seeds" and "walkers". Outside the box, a critical distance is defined, beyond which a "walker" starts to attach to a "seed". If this distance is reached, the movement stops, and the "walker" sticks to the "seed". The probability of adhesion is set to the maximum value to simulate diffusion.

The motion of individual particles or clusters is modeled as Brownian motion. The diffusion coefficient for a particle of radius r_i is given by the Stokes-Einstein equation:

$$D_i = \frac{k_B T}{6\pi\eta r_i} \tag{1}$$

where: - k_B is the Boltzmann constant,
- T is the temperature,
- η is the dynamic viscosity of the medium,
- r_i is the radius of the cluster.

The position ($x_i(t)$) of each walker is updated using a discrete random walk:

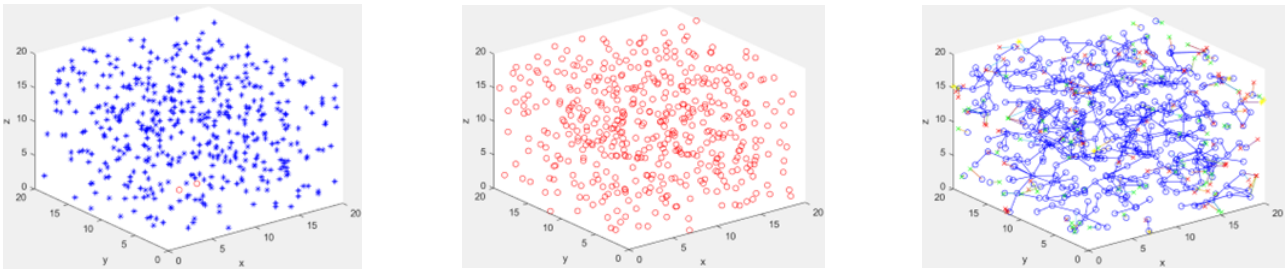
$$\mathbf{x}_i(t+\Delta t) = \mathbf{x}_i(t) + \sqrt{2D_i\Delta t}\cdot\mathbf{R} \tag{2}$$

where R is a random unit vector representing isotropic diffusion.

When a walker reaches a distance ϵ from an existing cluster, it adheres irreversibly. The aggregation rule follows:

$$\| \mathbf{x}_i - \mathbf{x}_j \| \leq \mathrm{T} \tag{3}$$

Cluster formation occurs when condition (2) is met. It means all "walkers" move towards the "seeds" and combine into a cluster. Clusters also join when two "walkers" exceed the critical distance between each other. Figure 1 shows the step-by-step construction of the model. All parameters, such as particle radius, critical distance, number of "seeds" and "walkers", their steps, box size, adhesion probability, and type of movement, can be adjusted. The structure modeling is implemented using MATLAB.



a – "Walkers" and "Seeds" *b* – "Seeds" *c* – Final model in MATLAB

Fig. 1 – I llustration of the model construction. The "seeds" are shown in red, and the "walkers" in blue. Gradually, all the "walkers" merge with the "seeds" and form clusters.

To construct a periodic structure, it is necessary to separate the connections near the walls of the box. To build correct connections, the rules of projecting points in the cube onto its faces are applied. A macro has been created to implement the model in the finite element method (FEM) numerical simulation software – ANSYS. The script configures material parameters, defines element and cross-section types for modeling a beam in ANSYS, and then creates the mesh and graph for visualizing the model.

Special attention is given to setting up the stress field and applying boundary conditions. The strain values for the strain components: ε_{xx} has a non-zero value, while the other strains are set to zero. Load tables are created for each displacement component (UX, UY, UZ). Boundary conditions define the displacements for the nodes of the cube at its boundaries. The displacement tables specify the displacement values for each component UX, UY, UZ depending on the coordinates. These conditions allow modeling the deformation of the cube according to the specified strains (ε_{xx}, ε_{yy}, ε_{zz}, ε_{xy}, ε_{yz}, ε_{xz}), ensuring proper loading and analysis of the model in ANSYS. Figure 2 shows the block diagram of the algorithm implementation.

Based on the approach described above, we implemented deformation and load modeling in ANSYS. Using the created load tables and defined boundary conditions, it was possible to successfully reproduce a realistic aerogel microstructure. The next step is to analyze the stress results in the model.

The von Mises stress criterion was used to evaluate the stress-strain state. This criterion is an effective method for determining the strength conditions of a material under complex loads, since it takes into account the influence of all components of the stress state.

Next, the modeling results are presented, including the distribution of von Mises stresses throughout the model volume. The zones of maximum stresses are also analyzed, which may indicate possible places of damage or material failure.

The results allow us to draw conclusions about the material's behavior under specified loading conditions and determine the key parameters that affect its strength and stability.

For FEM-based analysis, an APDL script translates DLCA-generated structures into ANSYS. The script configures material parameters, assigns element and cross-section types (BEAM188, CSOLID), and applies appropriate boundary conditions for stress analysis.

The material parameters used include:

- Young's modulus: 2.1×10^7 Pa
- Poisson's ratio: 0.3

Finite element modeling employs a two-node beam element with six degrees of freedom per node. Simulations are conducted for aerogel concentrations of 10% and 25%, with node and element counts summarized in Table I.

Table 1 – FE Models parameter for different concentration

Concentration, %	Nodes	Elements
25	7130	7994
10	2623	2648

4. Result of modelling. The results of DLCA-based modeling provide insight into the microstructure (fig. 3) and mechanical behavior of aerogels at different concentration levels (fig. 4). The generated aerogel structures exhibit fractal-like networks, consistent with experimental scattering data.

Stress distribution and displacement calculations reveal distinct mechanical responses for different aerogel concentrations:

10% concentration: The generated structure exhibits a highly porous network with long inter-cluster connections, leading to increased overall displacement under load. Maximum displacement is observed at the edges of the RVE, while stress distribution is relatively uniform.

25% concentration: Higher density results in more interconnected clusters, increasing stiffness and reducing overall displacement. Stress is concentrated in regions with high connectivity, indicating load-bearing paths within the structure.

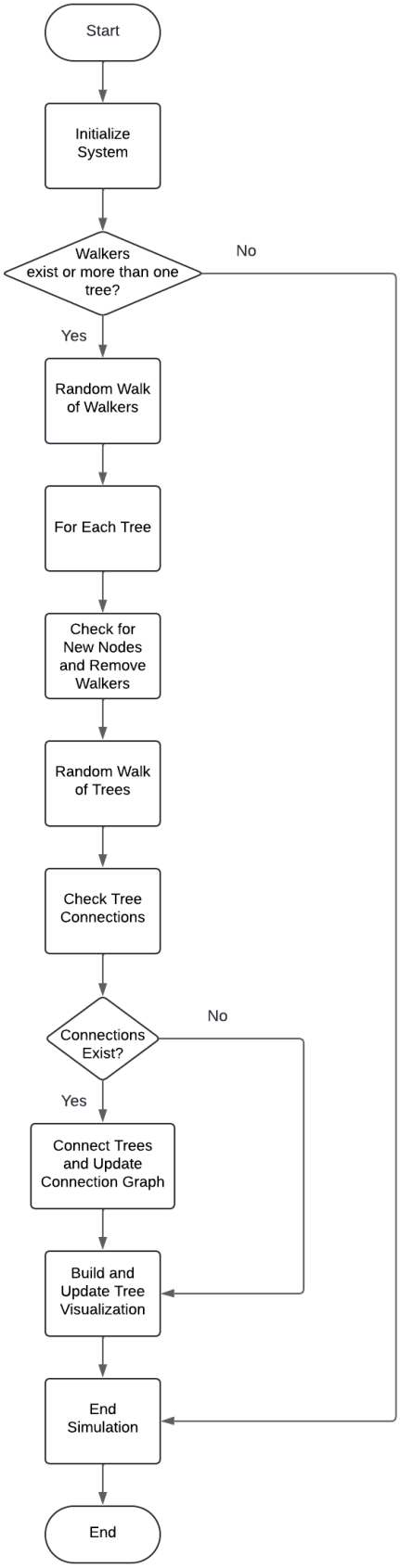
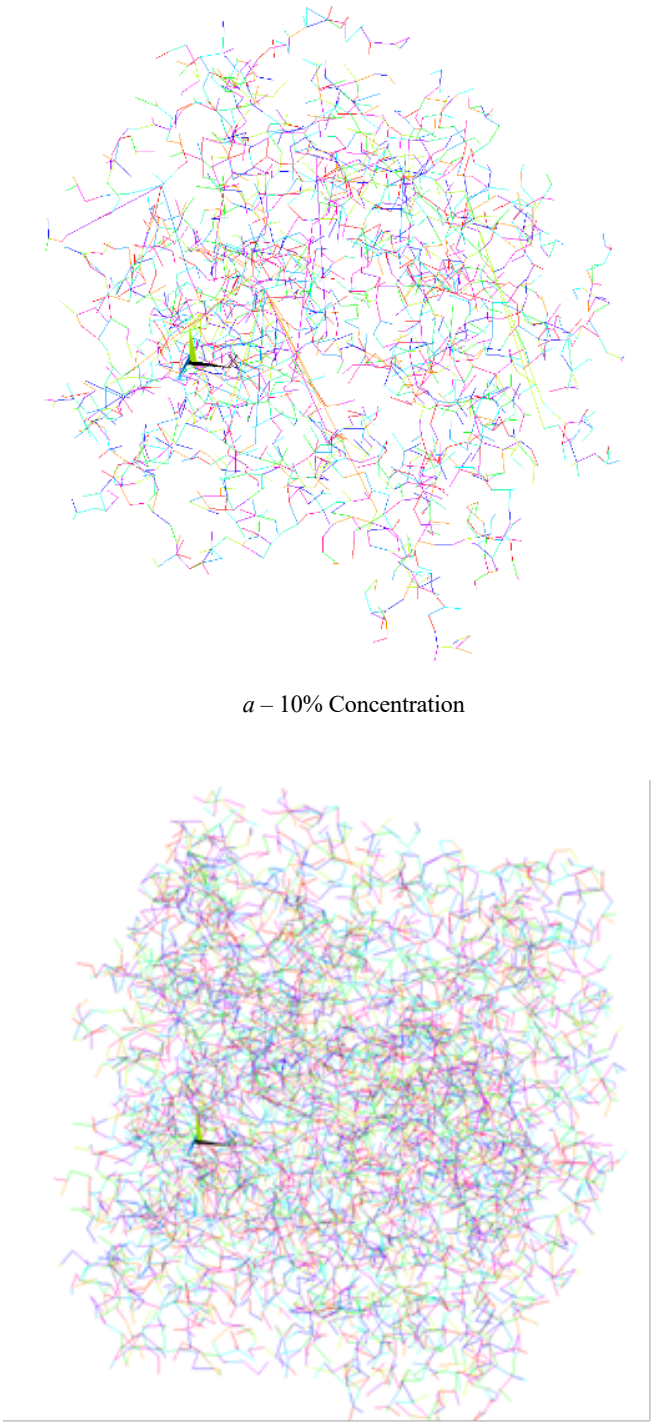


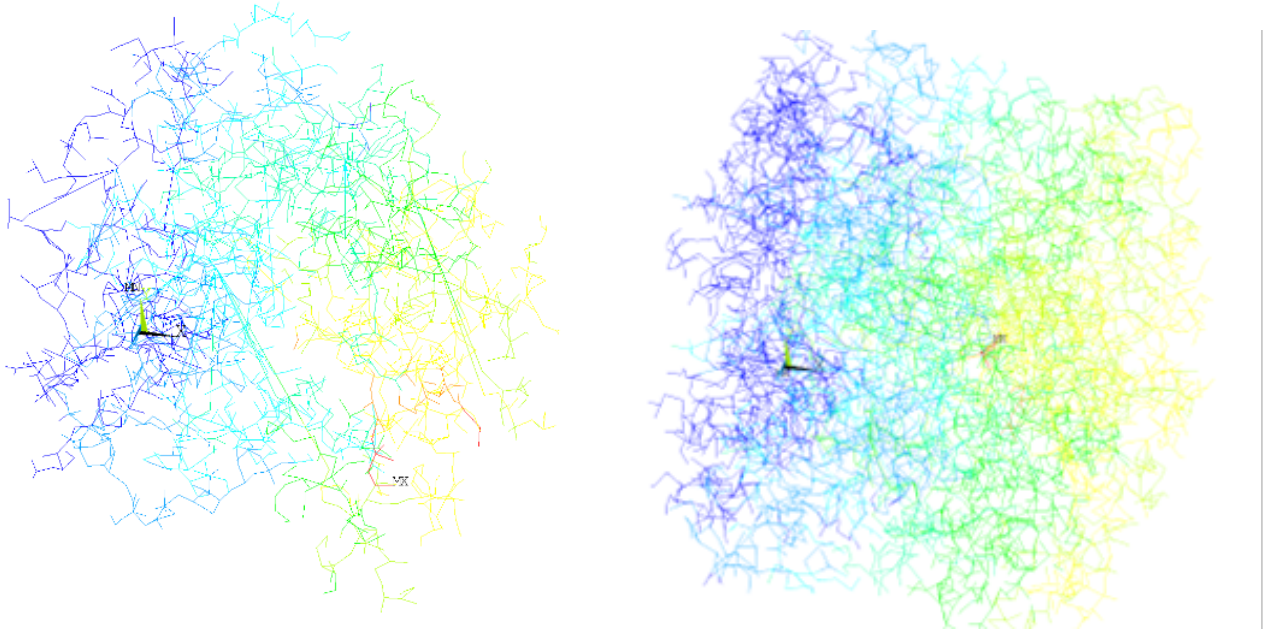
Fig. 2 – Block diagram of DLCA



a – 10% Concentration

b – 25% Concentration

Fig. 3 – Geometrical model: *a* – 10% Concentration, *b* – 25% Concentration



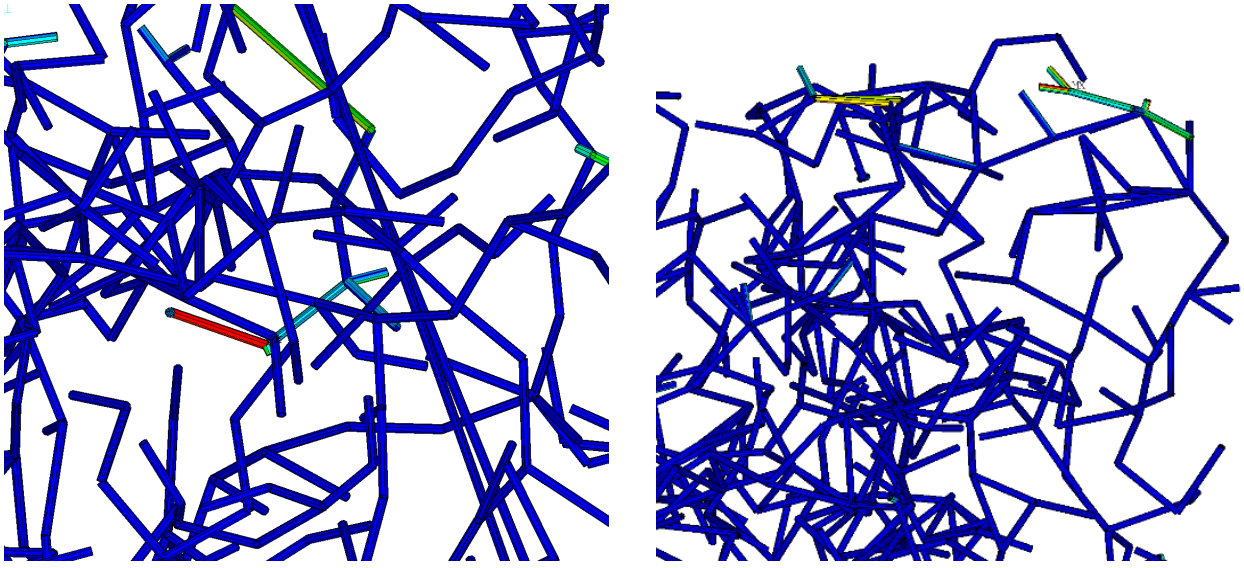
a – 10% Concentration *b* – 25% Concentration

Fig. 4 – Total displacement: *a* – 10% Concentration, *b* – 25% Concentration

Von Mises stress analysis highlights the correlation between structural density and mechanical response. The peak stress values increase with aerogel concentration due to the stronger inter-cluster connections. These results validate the DLCA-FEM approach for modeling aerogels, demonstrating its capability to capture structural and mechanical characteristics essential for material design and optimization (fig. 5).

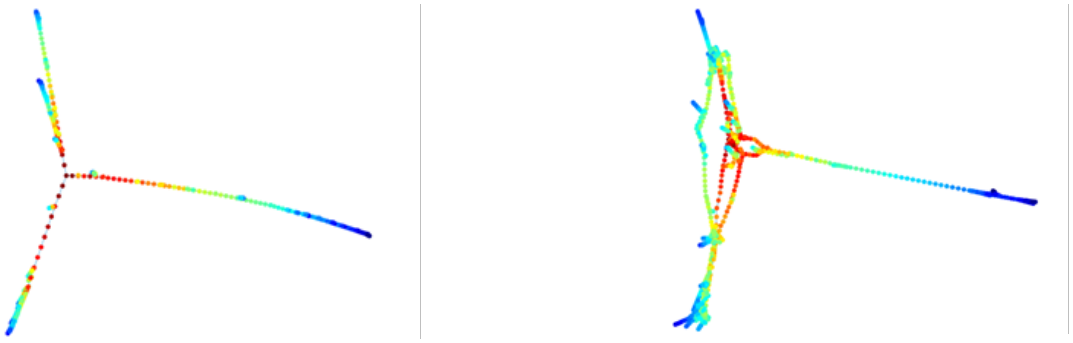
In the case of 10% concentration, the maximum total displacements are observed near the corner of the RVE, but if the concentration is higher, the maximum displacements are observed near the center of the RVE.

Also, in Figure 6 the two-dimensional graph represents the centrality metrics for both configurations.



a – 10% Concentration *b* – 25% Concentration

Fig. 5 – Von Mises stress distribution: *a* – 10% Concentration, *b* – 25% Concentration



a – 10% Concentration *b* – 25% Concentration

Fig. 6 – Centrality metrics: *a* – 10% Concentration, *b* – 25% Concentration

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6. Conclusions. This work developed algorithm and software for modeling the structure and mechanical behavior of aerogels.

It has been established algorithms that effectively simulate the formation of aerogel structures using the well-regarded DLCA approach.

A software tool has been created to execute the DLCA algorithms, enabling researchers to readily generate diverse aerogel structures for analysis.

The APDL scripts for translate the generated structures into finite element models compatible with ANSYS software is developed.

Initial calculations have been performed on these models to assess displacements and stresses under simple loading conditions, demonstrating the capability for mechanical behavior analysis.

Future work will involve:

- Expanding the analysis capabilities to encompass more complex loading scenarios and material properties.
- Further validation by comparing simulation results with experimental data on real aerogels.
- Exploring the applicability of this framework to model the structure and mechanics of other porous materials.

Overall, this work provides a powerful tool for researchers in the field of aerogel design and paves the way for further advancements in understanding and optimizing these materials.

References

1. *Abdusalamov, R., Scherdel, C., Itskov, M., Milow, B., Reichenauer, G., and Rege*, A. "Modeling and Simulation of the Aggregation and the Structural and Mechanical Properties of Silica Aerogels", J. Phys. Chem. B, vol. 125, pp. 1944–1950, 2021. https://doi.org/10.1021/acs.jpcb.0c10311
2. *Groß, J. and Fricke*, J. "Scaling of elastic properties in highly porous nanostructured aerogels0", Nanostruct. Mater., vol. 6, pp. 905–908, 1995. https://doi.org/10.1016/0965-9773(95)00206-5
3. *Gonçalves, W., Morthomas, J., Chantrenne, P., Perez, M., Foray, G., and Martin*, C. L. "Elasticity and strength of silica aerogels: A molecular dynamics study on large volumes", Acta Mater., vol. 145, pp. 165–174, 2018. https://doi.org/10.1016/j.actamat.2017.12.005
4. *Hrubesh*, L. W. "Aerogel applications", J. Non-Cryst. Solids, vol. 225(1), pp. 335–342, 1998. https://doi.org/10.1016/S0022-3093(98)00135-5
5. *Pierre, A. C. and Pajonk*, G. M. "Chemistry of aerogels and their applications", Chem. Rev., vol. 102(11), pp. 4243–4265, 2002. https://doi.org/10.1021/cr0101306
6. *Woignier T. et al.*, "Mechanical properties and brittle behavior of silica aerogels", Gels, vol. 1, pp. 256–275, 2015. https://doi.org/10.3390/gels1020256
7. *Borzęcka, N., Nowak, B., Pakuła, R., Przewodzki, R., and Gac*, J. "Cellular automata modeling of silica aerogel condensation kinetics", Gels, vol. 7, p. 50, 2021. https://doi.org/10.3390/gels7020050
8. *Pandit, P., Abdusalamov, R., Itskov*, M. et al., "Deep reinforcement learning for microstructural optimisation of silica aerogels", Sci Rep, vol. 14, p. 1511, 2024. https://doi.org/10.1038/s41598-024-51341-y. https://doi.org/10.1038/s41598-024-51341-y
9. *Rabbani, A., Babaei, M., Shams, R., Wang, Y., D. and Chung*, T. "DeePore: A deep learning workflow for rapid and comprehensive characterization of porous materials", Adv. Water Resour., vol. 146, p. 103787, 2020. https://doi.org/10.1016/j.advwatres.2020.103787
10. *Choubisa*, H. et al., "Interpretable discovery of semiconductors with machine learning", NPJ Comput. Mater., vol. 9, p. 117, 2023. https://doi.org/10.3390/gels7020050
11. *Brinker, C. J. and Scherer, G. W.* "Sol-Gel Science: The Physics and Chemistry of Sol-Gel Processing", Academic Press, 1990.
12. *Kwon, S. R. and Zhang*, X. "Mechanical characterization of aerogels using AFM", Mater. Lett., vol. 169, pp. 1–4, 2016.
13. *Jumper*, J. et al., "Highly accurate protein structure prediction with AlphaFold", Nature, vol. 596, pp. 583–589, 2021. https://doi.org/10.1038/s41586-021-03819-2
14. *Fricke, J., Tillotson*, T. "Aerogels: production, characterization and applications", Thin Solid Films – 1997 – №297 – С. 213-223 https://doi.org/10.1016/S0040-6090(96)09441-2
15. *Patil, S., Rege, A., Sagardas, Itskov, M., Markert, B.* "Mechanics of Nanostructured Porous Silica Aerogel Resulting from Molecular Dynamics Simulations", The Journal of Physical Chemistry B, vol. 121, pp. 5660-5668, 2017 https://doi.org/10.1021/acs.jpcb.7b03184

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