

Electronic supplementary information (ESI)

Code input parameters of the DLCA algorithm

The implementation of the diffusion-limited cluster-cluster algorithm (DLCA) for modeling silica aerogels was shown in Abdusalamov et al. [1]. In the following, information about the model parameters relevant to the developed artificial neural network (ANN) in the paper is provided. The DLCA model includes several parameters, namely, the number of seeds, the number of walkers, the step-size of the seeds, the step-size of the walkers, the particle radii (either having a constant value or provided as a distribution), the initial position of the seeds (either randomly chosen or carefully placed on grid lattice points). Since the initial positions of the seeds and the number of total particles (seeds and walkers) should not have an influence on the material properties, the authors chose to limit the input parameters for the ANN to four, namely, concentration (relative density), radius of the particles, step-size of the seeds and step-size of the walkers. The first two parameters can be controlled during the synthesis process, while the next two cannot, however, have an influence on the structural parameters of the final structure. The concentration (c) is defined as:

$$c = \frac{V_p}{V_L} = \frac{4\pi NR^3}{3L^3},$$

where, V_p , V_L , R and L denote the total volume of the particles, the total volume of the simulation box, the particle radius and the edge-length of the simulation box. N represents the number of particles. In order to vary the concentration, only the particle number N was changed, the box length L was kept constant. In a previous investigation, it was noticed that the step size has a major influence on the structural features as well as on the mechanical modeling [1]. This resulted in the choice of the other two parameters: the step size of the seeds and the walkers. Obviously, it is possible to train the ANN with even more input parameters. However, as the complexity of the model increases with each parameter, it becomes more difficult to correctly assess the influence of individual inputs. Since most algorithms follow an on-lattice method, a function was created for the movement of the particles that can switch between the off and on lattice. To move a particle, the position of a particle is changing by a shift $\mathbf{v} = a_i \mathbf{e}_i$ with $a_i \in [-s, s]$ where s is the step size either for a walker or seed particle. The factors a_i are equally distributed random numbers in the specified domain. Nevertheless, a distribution can also be provided.

Numerical determination of the fractal dimension

For the determination of the fractal dimension d_f , the described algorithm in [3] and [4] was used. In order to calculate d_f , the correlation function $g(r)$ can be determined by

$$\delta n = 24g(r)cr^2\delta r,$$

where r is the distance from an arbitrary particle center. δr denotes the increments in r for calculating the number of particles δn within the path $r + \delta r$. Using this relation, the accumulated mass of particles $m(r)$ is calculated as

$$m(r) = \int_0^r 24cr^2g(r) dr.$$

Additionally, the power law $m(r) \propto r^{d_f}$ holds. Thus, the fractal dimension d_f can be extracted by determining the slope of $m(r)$.

Determining the pore-size distribution

The pore-size distribution describes and quantifies the nature of the pore-space in the network. The volume fraction of spherical pores within a porous network is visualized over the pore radius. To determine the pore-size distribution, the algorithm presented in [2] was used.

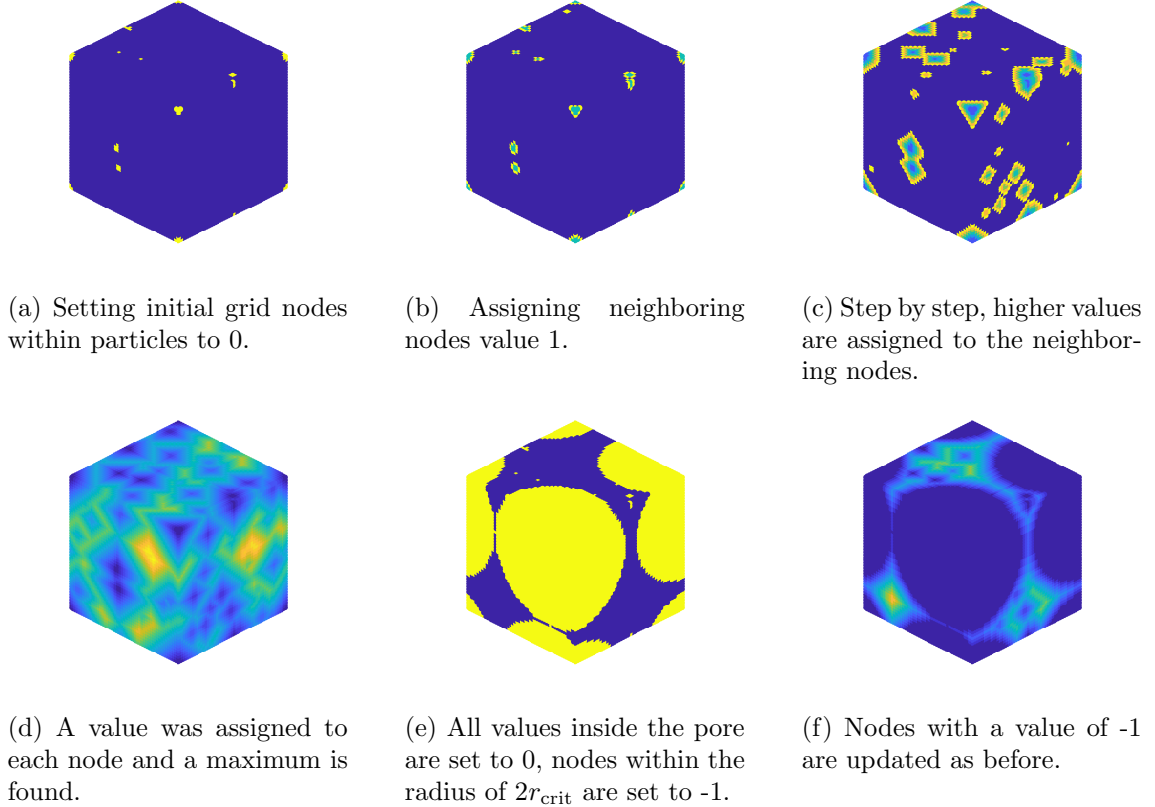


Figure S1: Illustration of the determination of the pore size distribution.

This is a grid search algorithm and works for a periodic RVE as follows (also, see Fig. S1):

1. Initially, the RVE is divided into a grid.
2. Each grid node is assigned a 0 if the node is inside a particle. All other nodes are assigned a -1.
3. In the next step, all nodes that have a value of -1 and are neighboring a node with the value 0 are identified. A value of 1 is assigned to these nodes.
4. Now all nodes that have a value of -1 and are neighboring a node with the value 1 are identified. A value of 2 is assigned to these nodes. This algorithm is now executed until no grid node has a value of -1.
5. The node with the maximum value is selected as a center point and the minimum periodic radius r_{crit} to the border of a particle is determined. All points inside and

on the border of this sphere are set to zero. All nodes that have a distance larger than r_{crit} but smaller than $2r_{\text{crit}}$ are set to -1 if their previous value was larger than 0.

6. Subsequently, the nodes with a value of -1 are updated as before.
7. This algorithm is repeated until the radius of the pore falls below 1.5 of the radius of the particles.
8. The pores can now be plotted and displayed in a histogram.

References

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