1.3 Stochastic Geometry in Homogenization

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The modern world has brought numerous technological advancements in a wide variety of fields, many of them dependent on the proper design of new materials, especially composites. First of all, the demand for specialized, high-performance materials is ever increasing as more and more use cases emerge; think of light-weight but sturdy wings for airplanes or degradation-resistant but efficiently functioning photovoltaic cells. The use of compound substances is almost ubiquitous here as many contrasting properties have to be combined. But also for less spectacular everyday life applications, we increasingly depend on a profound understanding of our materials across all ranges of size, since the scale at which we employ these materials is massive. The Hoover dam is a prominent and almost a century-old example, where the underlying geometric structure, like the steel beams inside the concrete or the microstructure of the concrete itself, has a tremendous impact on the stability of the entire object. Hence, a deeper understanding of not only the underlying materials but also the emerging macrostructures of these materials becomes necessary.

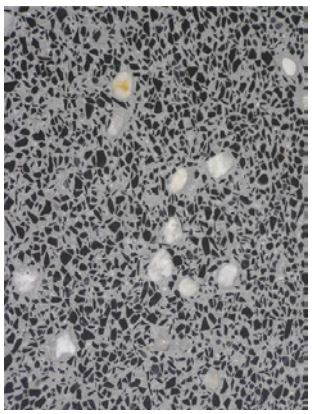


Fig. 1: *Polished concrete surface. Coarse black basalt is embedded in gray cement.*

A *concrete* example: Concrete is a mixture of cement, sand, and gravel, see Figure 1. At the same time, it is a perfect example of a porous medium: If not properly sealed, air and water, along with various aggressive chemicals, can penetrate deep into the material, slowly eroding it over time. This becomes problematic, for example, in bridges, sewage pipes, or dams, as the material eventually will erode even if sealed. To analyze the behavior of this mixture, one could try to track every single grain of sand and gravel and every pore in numerical simulations, but that would be way too complicated and time consuming. On the other hand, mathematical homogenization lets us simplify this problem by *averaging out* the tiny details of the material and look at it on a larger scale. Instead of focusing on each individual grain, we treat the concrete as if it were a single, uniform material with average properties. This method is extremely useful since

- it allows for simpler calculations as we only have to deal with one *averaged* substance now.
- In turn, this helps us to predict the macroscopic behavior of the compound material.

Such composite structures are common not only in engineered materials, but also in the natural world like volcanic rocks. Unfortunately, this *averaging out* proves to be far from simple. The effective physical properties of a composite material cannot be obtained by simple averaging over its constituents. Instead, we find that the underlying microscopic structure plays a vital role.

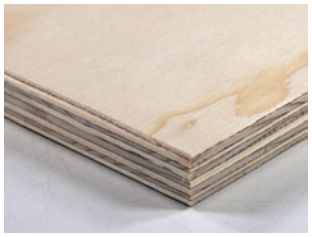


Fig. 2: *Plywood consisting of multiple horizontal wooden layers.* `https://commons.wikimedia.org/wiki/File:Spruce_plywood.JPG`

A brief introduction to homogenization

The goal of mathematical homogenization is to derive formulas that describe the macroscopic coefficients of the material in terms of their microstructure as well as the macroscopic equations that describe the material's effective behavior. It is important to emphasize that the macroscopic behavior may differ significantly from the microscopic behavior, particularly if certain effects dominate a complex system. A popular example for this is the dominance of friction between water and sand grains when water seeps into ground. This causes the microscopic Navier–Stokes equation to

turn into the simple Darcy equation. The prime example that is typically presented to students first is the stationary diffusion equation

$$-\nabla \cdot \left(a(x/\varepsilon)\nabla u^{(\varepsilon)}\right) = f, \tag{1}$$

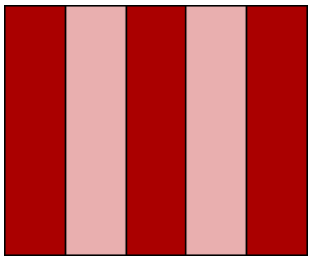


Fig. 3: Composite with non-isotropic a_{hom}. Given conductance a_1, a_2 on dark/light regions, the effective vertical conductance is $(a_1 + a_2)/2$, but $2/(a_1^{-1} + a_2^{-1})$ in the horizontal direction.

which—as the name suggests—can describe the diffusion of a substance in a carrier material. Also, it describes the flow of heat inside such a microstructure and other phenomena. Here, $a(x/\varepsilon) \geq 0$ denotes the conductivity of our heterogeneous medium in the point x, at scale ε of the microstructure, and f is some fixed function governing the heat source density. Given that a solution $u^{(\varepsilon)}$ exists for the partial differential equation (PDE), we study its behavior when ε tends to 0, i.e., when the scale of the microstructure becomes smaller and smaller. In this regard, we can formulate at least two goals, which are

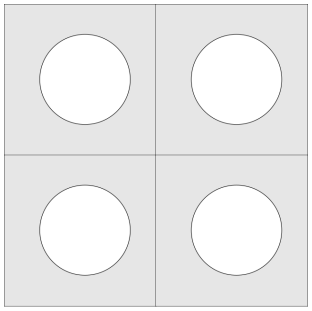
1. examining the convergence of $u^{(\varepsilon)}$ (in a suitable sense) to some $u := u^{(0)}$ as $\varepsilon \to 0$ and
2. identifying the governing PDE that is solved by u.

In contrast to the above-mentioned example of the Navier–Stokes to Darcy transition, the governing equation for the evolution of u remains the diffusion equation

$$-\nabla \cdot (a_{\text{hom}}\nabla u) = \tilde{f}, \tag{2}$$

where $\tilde{f}$ is proportional to f. The coefficient $a_{\text{hom}} \in \mathbb{R}^{d\times d}$ is the macroscopic mobility, which is now independent from x. This opens an opportunity for numerical simulations since the discretization of a uniform medium is much easier than the one for the original heterogeneous structures.

Finally, we note in this context that even if a is chosen to be a non-negative scalar, a_{hom} might turn out to be a non-isotropic matrix. Intuitively speaking, the flow may very well be dependent on the direction considered due to the underlying microstructure. This is evident in the cases of Figure 2 and Figure 3.



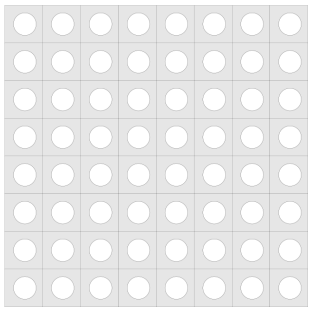


Fig. 4: Foam at scale $\varepsilon = 1$ (left) and $\varepsilon = 1/4$ (right) with the solid depicted in gray and the air bubbles in white

A small periodic example. We introduce a standard geometry model, which is used as an example for foams or concrete. We assume that inclusions into a carrying material are periodically repeating discs. Then, we can describe the conductivity of this material by choosing

$$a(x) := 1 - \chi_{B_{1/4}(\mathbb{Z}^d)}(x)\,,$$

where $B_{1/4}(\mathbb{Z}^d)$ is the set of all points with a distance less than $1/4$ to the next point in $\mathbb{Z}^d$ and $\chi_{B_{1/4}(\mathbb{Z}^d)}$ is the characteristic function of this set, see Figure 4. In this simple case, a_{hom} is a $d \times d$ matrix given by

$$a_{\text{hom}}(i,j) := \int_Y [e_i + \nabla w_i] \cdot [e_j + \nabla w_j]\mathrm{d}y\,, \tag{3}$$

where the $e_i \in \mathbb{R}^d$ are standard unit vectors and the $(w_i)_{i=1,\dots,d}$ are 1-periodic functions given as the solutions to the PDE $-\nabla \cdot [e_i + \nabla w_i] = 0$ in $Y = [-1/2, 1/2]^d \setminus B_{1/4}(0)$ with periodic boundary conditions. The latter are referred to as *cell solutions*. As can be seen from the formulas, a_{hom} is symmetric, but a calculation of the eigenvalues shows that it is typically not isotropic. With not too much effort, one can also prove that a_{hom} is positive semidefinite.

The realm of uncertainty: Stochastic homogenization

The above is a classical case of *periodic homogenization*. This makes sense for materials that have a predictable, often periodic structure, e.g., highly engineered materials or carefully planned out constructions. However, most real-world materials are far more erratic. Hence, the need to study *random microstructures* arises.

The setup is mostly the same. Let $U \subset \mathbb{R}^d$ be a bounded, open domain. To model the randomness, we need a stationary ergodic dynamical system, that is, a tuple $(\Omega, \mathcal{F}, \mathbb{P}, \tau)$ consisting of a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and an underlying family of shift operators $\tau = (\tau_x)_{x\in\mathbb{R}^d}$, $\tau_x : \Omega \to \Omega$. These must satisfy stationarity and ergodicity; meaning that the space is *homogeneous* and *averaging* over shifts. We assume that all randomness is driven by such a dynamical system. Consider a random closed set $G \subset \mathbb{R}^d$ satisfying $G(\tau_x\omega) = G(\omega) + x$ for almost every $\omega \in \Omega$ and every $x \in \mathbb{R}^d$. G serves as our random perforation. Thus, our new, random PDE is of the form

$$-\nabla \cdot \Big(a(\tau_{x/\varepsilon}\omega)\nabla u^{(\varepsilon)}(\omega)\Big) = f \qquad \text{in } U^{(\varepsilon)} := U\backslash(\varepsilon G(\omega)) \tag{4}$$

for some fixed realization $\omega \in \Omega$. A classical example can be constructed via point processes $\mathbb{X} \subset \mathbb{R}^d$ like in Figure 5 and Figure 6: Consider a stationary ergodic point process $\mathbb{X}$ and denote its distribution by $\mathbb{P}$. Choosing τ_x as the shift operator in $\mathbb{R}^d$ by $x \in \mathbb{R}^d$, $\tau_x\mathbb{X} := \mathbb{X} + x$, yields a stationary ergodic dynamical system. Then, we can consider its Boolean model with radius $r > 0$ as a perforation, that is, $G(\mathbb{X}) := B_r(\mathbb{X})$. However, even this most natural perforation model highlights a plethora of problems.

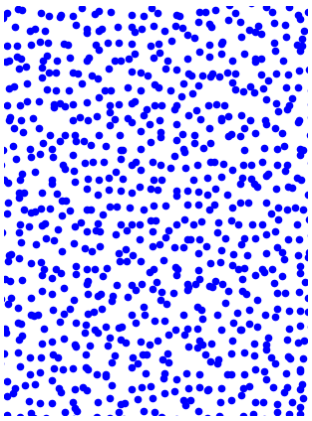


Fig. 5: *Random perforation based on a perturbed lattice*

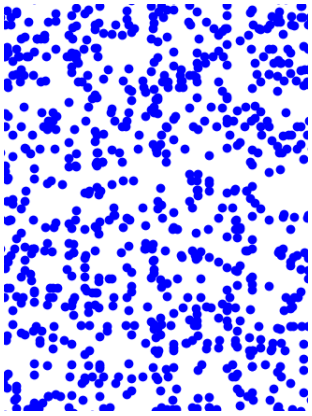


Fig. 6: *Boolean model of a Poisson point process*

Challenges. Stochastic homogenization presents several challenges, adding up to the already existing ones in periodic homogenization.

- Multiscale analysis: As before, capturing behavior at both microscopic and macroscopic scales necessitates careful asymptotic analysis.
- Convergence: Rigorously proving the convergence of the solutions $u^{(\varepsilon)}$ to the homogenized equation is often technically demanding. In the case of perforated domains, one often relies on extension operators.
- Randomness: Dealing with random coefficients requires probabilistic tools. However, completely new effects arise, which are unique to random geometries: arbitrarily large holes, sharp corners, thin tubes of material and, in general, a lacking control over geometric features.

It is, therefore, prudent to gather what is known and how the periodic setting can be translated to the stochastic one. One key aspect is dealing with the cell solutions. For that, we need some notion of partial derivatives on the probability space Ω. This can be defined as the dynamical system $\tau = (\tau_x)_{x\in\mathbb{R}^d}$, which introduces a strongly continuous group action on $L^2(\Omega) \to L^2(\Omega)$ by virtue of $T_x f(\omega) := f(\tau_x\omega)$. Periodicity is replaced by ergodicity, and so the form of a_{hom} and the (supposed) limiting equation can be easily guessed. a_{hom} has the same form as in (3) with $Y := \{\omega \in \Omega \mid 0_{\mathbb{R}^d} \notin G(\omega)\}$, while the limiting equation should be of the form

$$-\nabla \cdot (a_{\text{hom}}\nabla u) = \theta f \qquad \text{in } U, \tag{5}$$

where $\theta = \mathbb{P}(Y) = \lim_{\varepsilon\to 0} |U^{(\varepsilon)}|/|U|$ is the average density of our perforated domain. However, two key issues become apparent: showing convergence of the $u^{(\varepsilon)}$ and the exact shape of a_{hom}. In the following, we will give some insights into these.

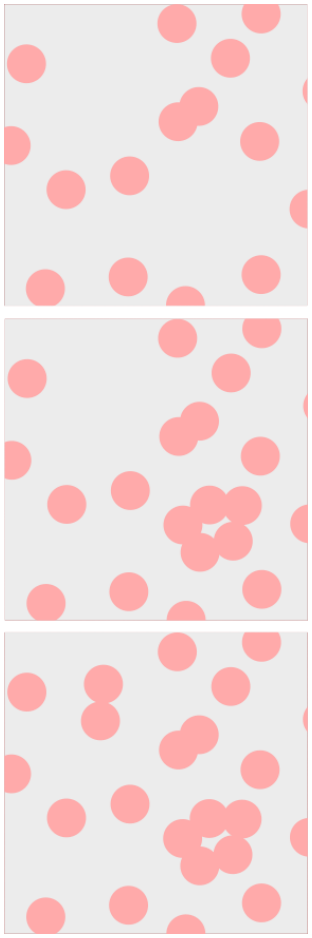


Fig. 7: *An approximation of an irregular perforation by regular ones*

Stochastic homogenization on irregularly perforated domains

While the homogenization of linear PDEs as introduced above is well understood, problems arise when the right-hand side f is replaced by a nonlinearity $f(u^{(\varepsilon)})$ or if nonlinear boundary conditions are supplemented on the interface between the union of all balls and their complements. In these cases, so-called *compactness results* as well as extension and trace operators become necessary. Unlike the periodic case, it is not possible to establish these statements for many random geometries, which is in part due to the already mentioned irregularities that may become arbitrarily bad locally (sharp corners, large holes, etc.).

In a joint project [1] between research group RG 1 *Partial Differential Equations* and Leibniz Group DYCOMNET *Probabilistic Methods for Dynamic Communication Networks*, we were able to alleviate this issue. We established an indirect homogenization scheme justifying the limit solution in (5). This is driven by a regularization of the irregular perforation as depicted in Figure 7. For each of the regularized domains $G^{(n)}$, we are able to homogenize the corresponding equation (4), arriving at a homogenized limit $u_n^{(\varepsilon)} \to u_n$ with corresponding limit equation. Then, we were able to establish $u_n \to u$ as $n \to \infty$, where u solves (5). The situation is depicted in Figure 8.

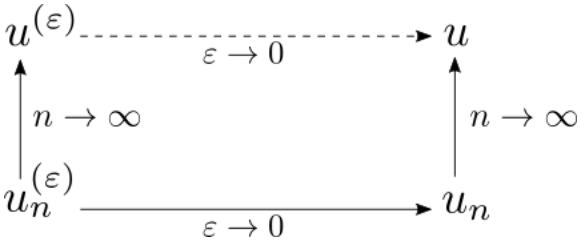


Fig. 8: *Convergences of the various solutions to (4) and (5) under regularization ($n \to \infty$) and microscale ($\varepsilon \to 0$). The dotted arrow is not known in general.*

Furthermore, this diagram is commutative in all cases where classical, direct homogenization results are available. Interestingly, our procedure requires $a_{\text{hom}} > 0$, i.e., a strictly positive definite a_{hom}—a requirement that is automatically fulfilled in the periodic case but may fail in the stochastic one.

Zero conductivity models

As previously mentioned, the shape of a_{hom} is highly dependent on the underlying stochastic model. It is difficult to calculate its exact shape even in the periodic case and regularity remains unclear in the stochastic one. This question marks the topic of our other collaborative project [2]. We study the pathological case of connected, albeit non-conductive random domains. As previously mentioned, this is a peculiarity of stochastic geometries. We move to a discrete lattice for simplicity, but the model and all equations easily translate to a continuous setting of a channel network. We constructed a stationary ergodic $\mathbb{Z}^d$-lattice model featuring $a_{\text{hom}} = 0$. Furthermore, for any fixed

volume fraction, the model can be tweaked to exceed that density. In other words, even though the material looks arbitrarily close to a solid block on a microscopic scale, the random perforations are aligned in such a way that the resulting macroscopic structure is non-conducting. To that end, we essentially exploit the following idea: elongating edges retains connectivity but may decrease conductivity. Performing this modification on a suitable percolation model generates a lattice as in Figure 9. We briefly sketch the model for $d = 2$. It is based on the randomly stretched lattice, which is a two-stage random lattice. Given $p, q \in (0,1)$, we first generate independent, identically distributed geometric random variables $N_i^{(x)}, N_j^{(y)}$, $i, j \in \mathbb{Z}$, with $\mathbb{P}(N_0^{(x)} \geq l+1) = q^l$. Then, an edge $(i,j) \leftrightarrow (i+1,j)$ is open with probability $p^{N_i^{(x)}}$ (and analogously $(i,j) \leftrightarrow (i,j+1)$ with $p^{N_j^{(y)}}$). It was proved in [3] that this lattice model percolates for $p > 1/2$ and q sufficiently small, i.e., it contains an infinite cluster of open edges. To establish zero conductivity, we now elongate these edges. Instead of having length 1, we stretch edges of the form $(i,j) \leftrightarrow (i+1,j)$ to have length $\mathcal{S}(N_i^{(x)})$, where

$$\mathcal{S}(N) := \lceil q^{-N(1-\sigma)} \rceil, \quad N \in \mathbb{N},$$

and $\sigma \in (0,1)$ is chosen such that $q^\sigma > p$. Doing the same for vertical edges, we obtain an elongated lattice similar to Figure 10. Since $\mathbb{E}[S(N_0^{(x)})] < \infty$, we may stationarize the modified lattice to obtain a stationary ergodic model on $\mathbb{Z}^2$. To ensure that a given fraction of edges is open, we may *fill up* blocks where $N_i^{(x)}$ and $N_j^{(y)}$ are low. This results in Figure 9. To establish $a_{\mathrm{hom}} = 0$, we rely on a variational formulation of (3), that is, almost surely

$$e_1^{\mathrm{t}} a_{\mathrm{hom}} e_1 = \lim_{n\to\infty} \inf_{V \in \mathcal{D}_n} \frac{1}{2} \sum_{z,\tilde{z} \in [0,n]^2 \cap \mathbb{Z}^2 \,:\, z \sim \tilde{z}} |V(\tilde{z}) - V(z)|^2,$$

with $e_1 = (1,0)^{\mathrm{t}} \in \mathbb{R}^2$, is the first standard unit vector and test function space $\mathcal{D}_n$ consisting of functions $[0,n]^2 \to \mathbb{R}$ taking values 0 on the left and 1 on the right of the box. Here, $z \sim \tilde{z}$ denotes that the summation is only done over open edges $z \leftrightarrow \tilde{z}$ (in the elongated lattice). Control over the probabilistic behavior of the lattice allows us to minimize the expression above, yielding $a_{\mathrm{hom}} = 0$.

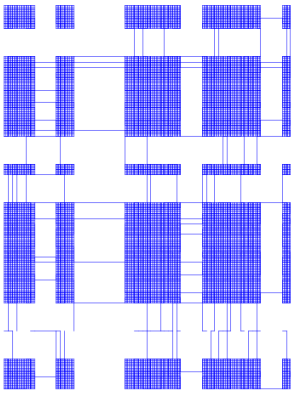


Fig. 9: *A connected lattice model featuring no conductance*

Conclusions and outlook

In our group collaboration between RG 1 and LG DYCOMNET, we were able to combine our expertise in homogenization and stochastic geometry to provide new models and methods for examining random materials via stochastic homogenization as a rigorous and versatile approach to understanding and modeling the behavior of systems in random media. By replacing detailed, computationally expensive microscopic models with effective macroscopic descriptions, this enables the analysis of complex systems with improved efficiency. As such, we strive to prove direct homogenization schemes for a wider class of models as well as to gain a better understanding of the effective conductivity in specific cases.

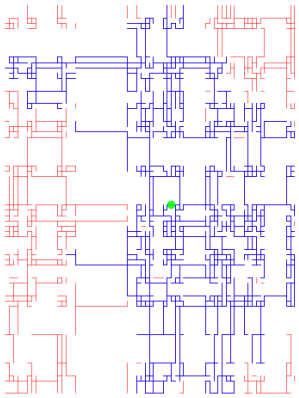


Fig. 10: *A connected lattice model featuring no conductance*

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