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Nanoionic Particle Composite Homogenization

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Nanoionic Particle Composite Homogenization

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Abstract

This project analyzes the effective conductivity of a material where the background conductivity of a substrate material is enhanced by the presence of nonconducting embedded particles. The averaged effective conductivity is derived using homogenization. The averaging is applied to several test examples, then to the material with particles embedded. The main interest is how various particle arrangements effect the overall conductivity.

Introduction

All models of physical phenomena make assumptions to simplify the models. For instance, a material is often assumed to be uniform, so that its properties apply evenly throughout. This allows us to take some physical quantity inherent in the material to be constant when in fact the quantity varies spacially. For example, the conductivity σ of a material is often taken to be constant.

Real-world materials are rarely so simple. Conductivity, and other properties, may not be constant throughout the entire material. In general, it is a function $\sigma(\mathbf{x})$ of position. This function may be complicated and difficult to analyze. It is useful to, roughly speaking, take an average value of σ, represented a constant matrix. This way, our models become easier to apply and understand. But how do we take the average of a complicated, possibly not explicitly known, function so that we don't lose too much information?

The answer lies in *homogenization*. We first define a physical quantity such as conductivity σ, by a system of partial differential equations with periodic boundary conditions on the unit square. This represents the problem on a small part of the domain– *microscale problem*. We use this to take averages, which we can apply to the problem on the whole domain– *macroscale problem*. This averages are called the *homogenziation coefficients*. In this report we apply homogenziation techniques to a material where conductivity is defined using a physically meaningful PDE system, described as follows.

Let U be a bounded, open set. This will be our macroscale domain, to represent our material. We consider the microscale periodically as follows. Let Q be the unit square in $\mathbb{R}^2$. Let $P \subset Q$ be some collection of disks, representing particles in our material, and set $Q^* = Q - P$. Physically Q^* is the substrate or background material surrounding the particles. The non-conducting particles affect how current flows through the material, in a phenomenon called the work function mismatch. A more detailed description of the physics behind the problem can be found in Fish et al (2012).

We want our electric potential v to have a voltage increase of 1 in the vertical direction over Q^*, and we want v periodic in the horizontal direction.

The microscale problem, defined over Q^*, is thus

$$\nabla \cdot (\sigma \nabla v) = 0 \qquad y \in Q^* \tag{1}$$
$$v(y_1, 0) = 0 \qquad 0 \leq y_1 \leq 1 \tag{2}$$
$$v(y_1, 1) = 1 \qquad 0 \leq y_1 \leq 1 \tag{3}$$
$$v \text{ periodic horizontally over } Q^* \tag{4}$$
$$\partial_n v = 0 \qquad y \in \partial P \tag{5}$$

where σ is the conductivity of the material, defined by $\sigma = e^{-\psi}$. Here ψ is a dimensionless potential over the material, defined as the solution to the following problem

$$\triangle \psi = \frac{1}{2\lambda^2}(1 - e^{-\psi}) \quad y \in Q^* \tag{6}$$
$$\psi = \psi_0 \quad x \in \partial P \tag{7}$$
$$\psi \text{ periodic} \quad y \in Q^* \tag{8}$$
$$\tag{9}$$

The particles in P are not charged. ψ_0 is a given constant describing the dimensionless potential on the surface of a particle. λ, also a given constant, is the Debye length of the material. When λ is small, the particle has little effect on the potential in the material. When λ is large, the particle has a much greater effect, leading to much stronger conductivity.

Notice that this second problem is nonlinear, making σ difficult to solve. We homogenize this second problem to find average values for σ. This turns the first problem into a linear problem with constant coefficients on the macroscale domain Ω. The details of the homogenization are in the section 2.

In section 3, we look at some test cases to introduce the process of homogenization, and how we analyze current flow. In section 4, we compute the homogenization coefficients in a few different situations, looking at how differnt arrangements of particles, particle sizes, and values of λ affect current flow. We then determine which situtation is optimal for maximizing current flow.

Homogenization

The following is a well known derivation of the homogenization coefficients that can be found in Evans (2010).

Let U be an open bounded subset of $\mathbb{R}^2$, with smooth boundary ∂U. Consider the following system:

$$Lu := \sum_{i,j=1}^{2} \left(a^{ij} \left(\frac{x}{\epsilon} \right) u^{\epsilon}_{x_i} \right)_{x_j} = f \quad x \in U \tag{10}$$

$$u^{\epsilon} = 0 \quad x \in \partial U. \tag{11}$$

Here the functions $f : U \to \mathbb{R}$ and $a^{ij} : U \to \mathbb{R}$ for $i, j \in \{1, 2\}$ are given. For convenience, we will assume the *uniform ellipticity condition* on a^{ij}. In other words, we assume that there exists a constant $\theta > 0$ such that

$$\sum_{i,j=1}^{2} a^{ij}(y) \xi_i \xi_j \geq \theta |\xi|^2$$

for all $y, \xi \in \mathbb{R}^2$. We also assume that a^{ij} is periodic over the unit square Q, which will represent our microscale. Note that this means that the functions $a^{ij}\left(\frac{x}{\epsilon}\right)$ in (10) are oscillating rapidly for small $\epsilon > 0$ over our macroscale U. Our goal is to determine how this affects the solution u^{ϵ}, as our length scale $\epsilon \leftarrow 0$.

Assume that there is some function $u : U \to \mathbb{R}$ such that $u^{\epsilon} \to u$ as $\epsilon \to 0$ in some suitable sense. We will attempt to find some PDE system that u satisfies. To do this, we begin by assuming that u^{ϵ} admits a *two-scale expansion* as follows

$$u^{\epsilon}(x) = \sum_{i=0}^{\infty} \epsilon^i u_i(x, x/\epsilon) \tag{12}$$

where $u_i : U \times Q \to \mathbb{R}$ for each i. Each term $u_i = u_i(x, y)$ is thought of as a function of two variables. The variable x in the domain U is called the *macroscale variable*, and y in Q is the *microscale variable*. Note that the u_i terms are periodic in y. We will plug the expansion in (2.3) into the PDE problem in (2.1-2), and solve a series of problems from equating the coefficients of powers of ϵ.

Suppose we had a differentiable function $w(x, y)$. Let $v(x) = w(x, x/\epsilon)$. Using the chain rule, we see that $\frac{\partial}{\partial x_i} v = \frac{\partial}{\partial x_i} w + \frac{1}{\epsilon} \frac{\partial}{\partial y_i} w \equiv \left(\frac{\partial}{\partial x_i} + \frac{1}{\epsilon} \frac{\partial}{\partial y_i} \right) w$. We find that

$$L = \frac{1}{\epsilon^2}L_1 + \frac{1}{\epsilon}L_2 + L_3 \tag{13}$$

where $L_1, L_2,$ and L_3 are defined as follows

$$L_1 w = \sum_{i,j=1}^{2} \left(a^{ij}\left(\frac{x}{\epsilon}\right) w_{y_i}\right)_{y_j} \tag{14}$$

$$L_2 w = \sum_{i,j=1}^{2} \left(a^{ij}\left(\frac{x}{\epsilon}\right) w_{x_i}\right)_{y_j} + \left(a^{ij}\left(\frac{x}{\epsilon}\right) w_{y_i}\right)_{x_j} \tag{15}$$

$$L_3 w = \sum_{i,j=1}^{2} \left(a^{ij}\left(\frac{x}{\epsilon}\right) w_{x_i}\right)_{x_j} \tag{16}$$

We now plug the expansion in (12) into the PDE system (10-11) and combine like powers of ϵ, as follows

$$\frac{1}{\epsilon^2}L_1 u_0 + \frac{1}{\epsilon}(L_1 u_1 + L_2 u_0) + (L_1 u_2 + L_2 u_1 + L_3 u_0) + O(\epsilon) = f$$

where $O(\epsilon)$ refers to terms involving positive powers of ϵ. Since f is not dependent on ϵ, we can use this equation to deduce

$$L_1 u_0 = 0 \tag{17}$$

$$L_1 u_1 + L_2 u_0 = 0 \tag{18}$$

$$L_1 u_2 + L_2 u_1 + L_3 u_0 = f \tag{19}$$

First, we find that $u_0(x, y)$ solves $L_1 u_0 = 0$, and is periodic over Q in y. Since we assumed this problem satisfied uniform ellipticity, u_0 must satisfy the maximum and minimum principles: the maximum and minimum values of u_0 must be found on the boundary. But our boundary conditions are periodic in both directions, so u_0 must be constant on the boundary. As a result, it is constant in y. Thus $u_0 = u(x)$ is a function only on the macroscale.

Now we apply (15) and (18). Since u_0 is constant in y, the partial derivatives with respect to y must be 0. We thus find

$$L_1 u_1 = -\sum_{i,j=1}^{2} a^{ij}(y)_{y_j} u_{x_i} \tag{20}$$

We now apply separation of variables. For $i = 1, 2$, let $\chi^i = \chi^i(y)$ be a solution to the *corrector problem:*

$$L_1 \chi^i = -\sum_{j=1}^{2} a^{ij}(y)_{y_j} \quad y \in Q \tag{21}$$

$$\chi^i \text{ periodic over } Q \tag{22}$$

To show that this has a solution, we apply the *Fredholm alternative.* This theorem states that either the nonhomogenous elliptic PDE problem must have a solution, or the homogenous problem has a nontrivial solution. If you take the integral over Q of both sides, we see that the right-hand side has integral 0. So we know a nonhomogenous solution exists. From periodicity, we know that this solution is unique up to an added constant.

We can now represent u_1 by

$$u_1(x, y) = \sum_{i=1}^{2} \chi^i(y) u_{x_i}(x) + \tilde{u}_1(x), \tag{23}$$

where $\tilde{u}_1$ is an arbitrary function only of x.

Lastly, we consider (19), rewritten as follows

$$L_1 u_2 = f - L_2 u_1 - L_3 u_0 \tag{24}$$

In order for (24) to have a solution which is periodic over Q in y, the integral of the right hand side over Q must be 0. This gives us

$$\int_Q (L_2 u_1 + L_3 u_0) dy = \int_Q f dy = f, \tag{25}$$

since f is a function only of x and Q has area 1.

It turns out that

$$\int_Q L_2 u_1 dy = \sum_{i,j,k=1}^{2} \left(\int_Q a^{jk}(y) \chi^i_{y_k}(y) dy \right) u_{x_i x_j}$$

Recall that by assumption, u was the limit of u^ϵ as $\epsilon \to 0$. Using the expansion from (2) we see that $u = u_0$. From (10), we find that

$$\sum_{i,j=1}^{2} \left(\int_Q a^{ij}(y) - \sum_{k=1}^{2} a^{jk}(y) \chi^i_{y_k}(y) dy \right) u_{x_i x_j} = f$$

This brings us to our goal of finding a PDE system satisfied by u:

$$\sum_{i,j=1}^{2} \bar{a}^{ij} u_{x_i x_j} = f \quad x \in U \tag{26}$$

$$u = 0 \quad x \in \partial U \tag{27}$$

where

$$\bar{a}^{ij} = \int_Q \left[a^{ij}(y) - \sum_{k=1}^{2} a^{jk}(y) \chi^i_{y_k}(y) \right] dy \tag{28}$$

define the *homogenized coefficients* and the χ^i solve the corrector problem.

Test Examples

Now that we know how to find the homogenization coefficients, we can use this information to solve our problem. First, we look at three similar problems as test cases.

Analytic Example

Before limiting our focus to situations that necessitate numerical computations, it is useful to consider a simple example where we can apply the derivation of the previous section exactly. Suppose the conductivity in our material are defined according to Figure 1, where σ_1 and σ_2 are given constants.

According to a result from Hashin and Shtrikman (1962), the effective conductivity σ_{eff} applied to current flowing through this material in any direction is such that

$$\frac{2\sigma_1\sigma_2}{\sigma_1\sigma_2} \leq \sigma_{eff} \leq \frac{\sigma_1 + \sigma_2}{2}$$

Notice that if the current flows horizontally, we consider the two conductivities to be in parallel. Thus we would expect the effective conductivity in this case to be $\frac{\sigma_1+\sigma_2}{2}$. On the other hand, if the current flows vertically the conductivities will be in series, and from physics we expect the effective conductivity to be $\frac{2\sigma_1\sigma_2}{\sigma_1\sigma_2}$. Using the notation from the previous section, we expect these values to be $\bar{a}^{11}$ and $\bar{a}^{22}$ respectively.

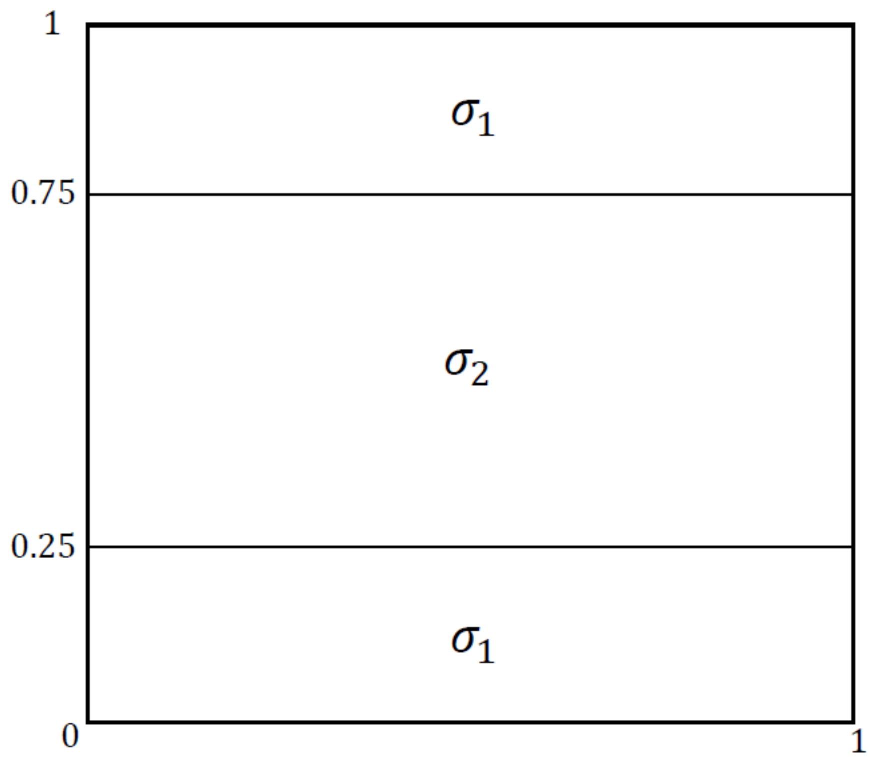


Figure 1: Diagram displaying the conductivity over this material, defined as a step function

We let $a^{11}(y) = a^{22}(y) = \sigma(y)$ to be the function in the figure, and we let $a^{12}(y) = a^{21}(y) = 0$. The resulting PDE system is uniformly elliptic, and our homogenization coefficients are thus

$$\begin{aligned}
\bar{a}^{11} &= \int_Q \sigma(y)(1 - \chi^1_{y_1})dy \\
\bar{a}^{12} &= -\int_Q \sigma(y)\chi^1_{y_2}dy \\
\bar{a}^{21} &= -\int_Q \sigma(y)\chi^2_{y_1}dy \\
\bar{a}^{22} &= \int_Q \sigma(y)(1 - \chi^2_{y_2})dy
\end{aligned}$$

where χ^1 and χ^2 are solutions to the corrector problem for this material

$$\begin{aligned}
(\sigma(y)\chi^1_{y_1})_{y_1} + (\sigma(y)\chi^1_{y_2})_{y_2} &= 0 \\
(\sigma(y)\chi^2_{y_1})_{y_1} + (\sigma(y)\chi^2_{y_2})_{y_2} &= (\sigma_2 - \sigma_1)(\delta(y_2 - 0.25) - \delta(y_2 - 0.75)) \\
\chi^1, \chi^2 \text{ periodic}
\end{aligned}$$

Here, δ is the Dirac delta distribution, which serves as the weak derivative of the unit step function.
From inspection, we see that χ^1 is any constant. One can find a solution for χ^2 that depends only on the vertical position

$$\chi^2 = \begin{cases} \frac{\sigma_2-\sigma_1}{\sigma_1}cy_2 + k & \text{if } y_2 \le \frac{1}{4}, \\ \frac{\sigma_2-\sigma_1}{\sigma_2}(1+c)(y_2 - \frac{1}{4}) + \frac{\sigma_2-\sigma_1}{4\sigma_1}c + k & \text{if } \frac{1}{4} < y_2 \le \frac{3}{4}, \\ \frac{\sigma_2-\sigma_1}{\sigma_1}c(y_2 - \frac{3}{4}) + \frac{\sigma_2-\sigma_1}{2\sigma_2}(1+c) + \frac{\sigma_2-\sigma_1}{4\sigma_1}c + k, & \text{if } y_2 > \frac{3}{4} \end{cases}$$

where k is arbitrary and $c = \frac{-\sigma_1}{\sigma_1+\sigma_2}$. From the integral formulas, our homogenization coefficients are as follows

$$A := \{\bar{a}^{ij}\} = \begin{bmatrix} \frac{\sigma_1+\sigma_2}{2} & 0 \\ 0 & \frac{2\sigma_1\sigma_2}{\sigma_1+\sigma_2} \end{bmatrix}$$

We conclude from this example that the homogenization process gives results that are consistent with what we know from physics. We now consider another example, which we solve computationally.

Conductivity Defined with no Particles

Suppose the conductivity in the material is defined in terms of the following step function. We will consider the following problem in $\mathbb{R}^2$

$$(a(y)u_{y_1})_{y_1} + (a(y)u_{y_2})_{y_2} = 0 \qquad y \in Q \tag{29}$$

subject to periodic boundary conditions. Here, Q is the unit square, and a is defined as follows

$$a(y) = \begin{cases} 2 & \text{if } y_1, y_2 < \frac{1}{4}, y_1, y_2 > \frac{3}{4}, \text{ or } \frac{1}{4} < y_1, y_2 < \frac{3}{4}, \\ 1 & \text{otherwise} \end{cases} \tag{30}$$

Again, the resulting system is uniformly elliptic. Our goal is to homgenize this problem, and find the solution on the macroscale. Specifically, we want a 4×4 matrix A of averaged conductivities such that

$$\nabla \cdot A \nabla v = 0 \qquad x \in \Omega \tag{31}$$

subject to appropriate boundary conditions, where v is the macroscale solution as the period of y approaches 0. Ω is the full domain of the material.

We find A as in the previous section.

$$\bar{a}^{11} = \bar{a}^{22} = \int_Q a(y)(1 - \chi(y)_{y_1})dy \qquad \bar{a}^{12} = \bar{a}^{21} = -\int_Q a(y)\chi(y)_{y_1}dy \tag{32}$$

Here, χ is again the solution to the corrector problem

$$\begin{cases} (a(y)\chi(y)_{y_1})_{y_1} + (a(y)\chi(y)_{y_2})_{y_2} = a(y)_{y_1} \\ \chi \text{ periodic on } Q \end{cases} \tag{33}$$

We make a few remarks. First, since a is a discontinuous function, it is clearly not differentiable in the classical sense. In all of the above equations, the partial derivatives of a are understood in a weak sense; we apply the Dirac delta distribution to simulate a jump. Also, observe that this problem is symmetric. Thus, it does not matter whether we take the partial derivative with respect to $y_1$or y_2 in either equation; y_1 was chosen arbitrarily. Finally, note that the corrector problem does not admit a unique solution, but all solutions differ only by a constant. Since we only use derivatives of in our

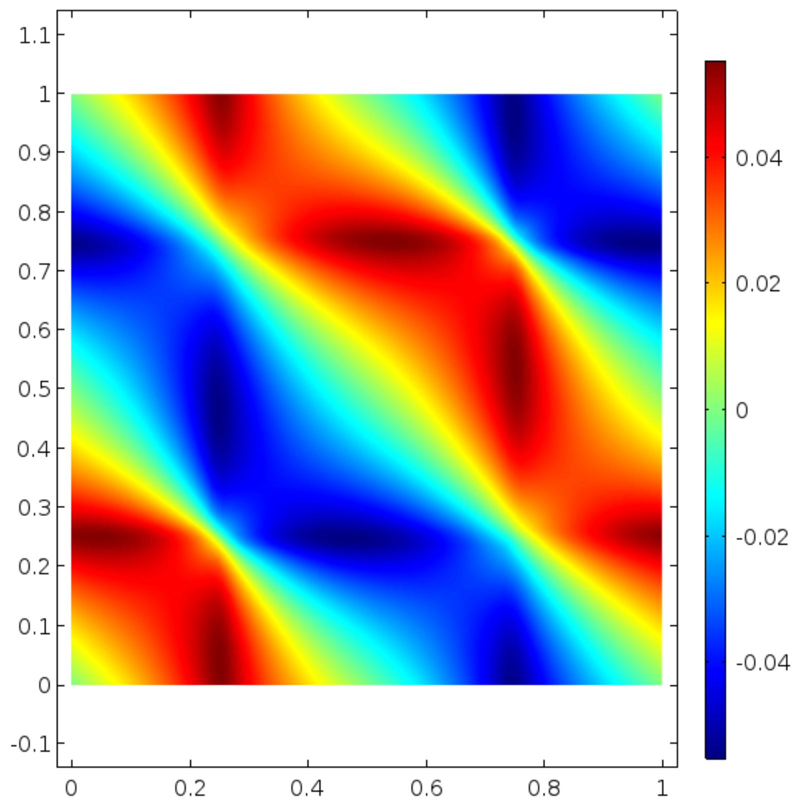


Figure 2: Approximation of χ in the second test example. The domain is the unit square Q

formulas for the coefficients, it does not matter which solution we use.

The entries of A were computed by numerically solving the corrector problem, and using the resulting solution to approximate the integrals. For this purpose, the *COMSOL Multiphysics* equation-based modelling software was used. The right-hand side of the cell problem was approximated using Gaussian pulse functions, each with a standard deviation of 0.01. Also, because this problem is only well-posed up to an added constant, we included the constraint $\int_Q \chi = 0$, fixing the average value of the solution to guarantee that it will converge.

The result of the computation of χ is shown in Figure 2. Using this solution and (32), we can compute A

$$A = \begin{bmatrix} 1.425 & -0.0798 \\ -0.0798 & 1.425 \end{bmatrix} \tag{34}$$

Note that since $a(y)$ is symmetric, A is a symmetric matrix. We apply this result to a specific example. Suppose the domain is a material, represented by Q, that is nonhomogenous. The conductivity across the material is defined on the microscale by a. We assume we have a voltage difference of 1 in the vertical direction across a period. We are interested in the *effective current* of the material, or the current across the homogenized material. We take the microscale problem and homogenize. The resulting macroscale problem is defined as

$$\begin{cases} \nabla\cdot A\nabla v = 0 & x \in Q \\ v(x_1, 0) = 0 & x_1 \in [0,1] \\ v(x_1, 1) = 1 & x_1 \in [0,1] \\ v(0, x_2) = v(1, x_2) & x_2 \in [0,1] \\ v_{x_1}(0, x_2) = v_{x_1}(1, x_2) & x_2 \in [0,1] \end{cases}$$

We can then evaluate the effective current by integrating the flux of v across the top of Q. In other words,

$$i_{eff} = \int_0^1 A\nabla v\cdot \hat{n} dx_1$$

In this example, we find that $i_{eff} = 1.425$. We note that this has the same numerical value as the value of A along the main diagonal.

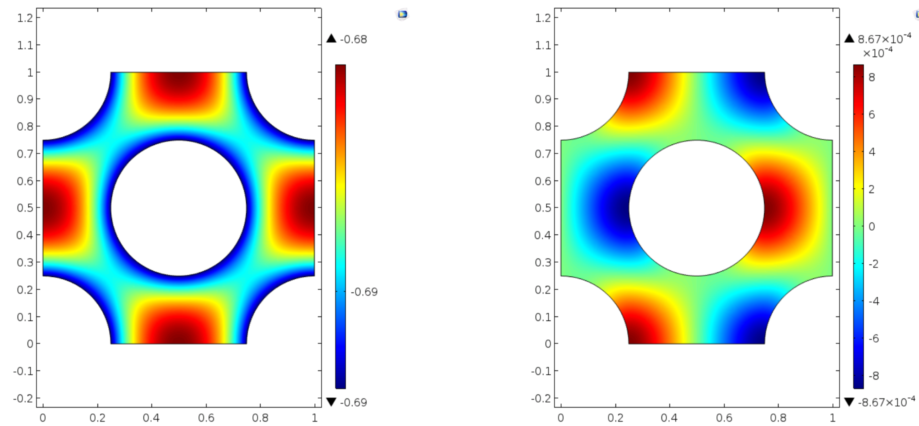
We can also consider current flowing in a general direction. Consider a general homogenization matrix A like the following

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$$

Then, assuming that $v \in C^2(\Omega)$ and thus $v_{x_1x_2} = v_{x_2x_1}$, the macroscale equation for voltage becomes

$$a_{11}v_{x_1x_1} + (a_{12} + a_{21})v_{x_1x_2} + a_{22}v_{x_2x_2} = 0 \tag{35}$$

Intuitively, the main diagonal entries in the matrix describe the strength of current flowing in the x_1 and x_2 directions, in that order. The off-diagonal



(a) Approximation of ψ (b) Approximation of χ

Figure 3: Solutions for ψ and χ for the third test example

elements represent a loss of conductivity resulting from the structure of the material. We see that this matrix is diagonally dominant, as the off-diagonal entries are fairly small. This is not surprising, as we would not expect a significant loss of current.

Two Particles in a Cell

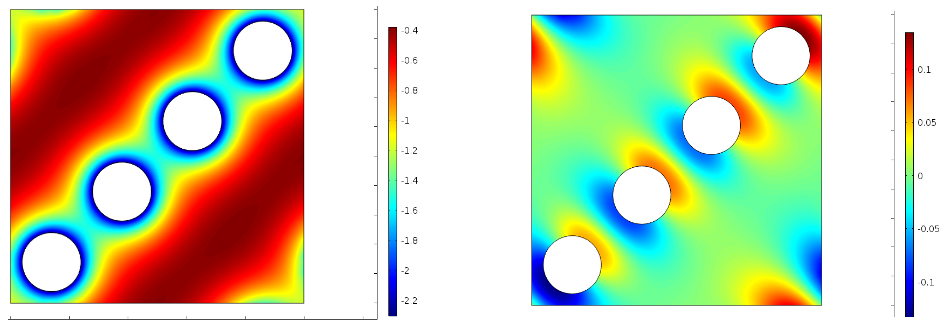
We examine another test case. Here we introduce particles, and we define conductivity in a way that is more physically meaningful. Let $a = e^{-\psi}$, where ψ is the solution to the following problem

$$\triangle\psi = \frac{1}{2\lambda^2}(1 - e^{-\psi}) \qquad y \in Q^* \tag{36}$$

$$\psi \text{ periodic} \tag{37}$$

$$\psi = -\ln 2 \qquad y \in \text{particle} \tag{38}$$

Suppose that on the microscale, each unit cell has two particles. Our unit cell will be centered at one particle, and a quarter of a particle will be at each corner. Each particle has radius $R = 0.25$. We use a Debye length $\lambda = 1$. We compute χ and solve for our homogenization matrix A as before. The approximate solutions for ψ and χ are in shown in Figure 3. We observe that ψ, and hence σ, is almost constant with this choice of λ.



(a) Approximation of ψ

(b) Approximation of χ

Figure 4: Solutions for ψ and χ for the particles arranged along the diagonal. The Debye length is $\lambda = 0.1$

We then find our matrix A to be

$$A = \begin{bmatrix} 1.21 & 0.002 \\ 0.002 & 1.21 \end{bmatrix} \tag{39}$$

Just as in the previous example, we find this matrix to be diagonally dominant, and thus find only a small loss of current, regardless of the direction of flow. The resulting material is highly conductive, particularly with this large choice of λ. The size of the particles in this example is larger than what we would usually consider, which also affects the data. In the next section, we begin examining cases more carefully.

Main Problem: Computations and Results

In this section, we look at various different orientations of particles inside the unit square, and analyze how the resulting current is affected. We also look at how changing the value of λ affects the current. We use five different values of λ for each case: 0.1, 0.316, 1, 3.16, and 10.

Particles Along a Diagonal

We consider a microscale cell with four particles. Each particle has a radius of 0.1, and they are arranged along the diagonal starting from the bottom-left and ending at the top-right. The setup is shown in Figure 4.

In this case, we use a value of $\psi = -\ln 10$ on the surface of the particles as a boundary condition. Otherwise, the PDE system remains the same as in the previous chapter. Table 1 contains the values of A for the different values of λ when the particles are arranged diagonally.

λ	0.1	0.316	1	3.16	10
a_{11}	2.693	5.284	7.912	8.644	8.733
a_{12}	0.2591	0.1370	0.0277	0.0032	3.24E-4
a_{21}	0.2590	0.1369	0.0277	0.0032	3.24E-4
a_{22}	2.693	5.284	7.912	8.644	8.733

Table 1: Entries of Matrix A for the particles arranged diagonally, using different values of λ. a_{ij} is the entry in row i and column j of A.

Since this problem is still symmetric, we find that A is again a symmetric matrix. As λ gets larger, so does the value of the effective current. The off-diagonal entries are small throughout, and become even smaller as λ becomes larger. We thus find that this arrangement of particles induces high conductivity, with very little loss of current moving in any direction.

Particles Arranged Horizontally

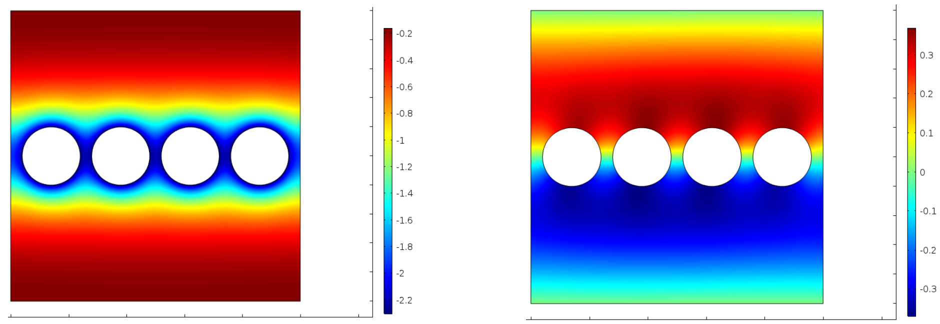
Our next case includes four particles arranged in a horizontal row in the middle of the cell. They all have an x_2 component of 0.5, and they are centered and equally spaced across the horizontal. This is shown in Figure 5.

Table 2 contains the entries in A for the different values of λ.

λ	0.1	0.316	1	3.16	10
a_{11}	2.222	4.246	7.252	8.535	8.722
a_{12}	0.0953	0.033	0.007	8.43E-4	8.65E-5
a_{21}	-0.5115	0.2260	0.402	0.071	0.0076
a_{22}	1.615	4.439	7.647	8.605	8.729

Table 2: Entries of Matrix A for the particles arranged horizontally, using different values of λ.

There are a few observations to make for this case. First, we observe that A is no longer a symmetric matrix. This should be expected, because



(a) Approximation of ψ

(b) Approximation of χ

Figure 5: Solutions for ψ and χ for the particles arranged horizontally. The Debye length is $\lambda = 0.1$

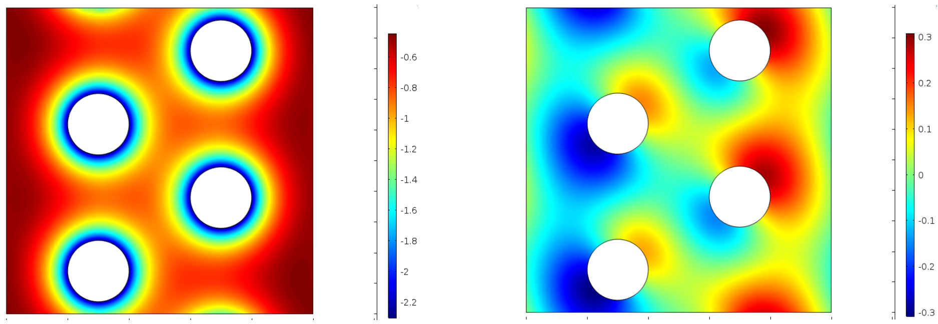
the problem no longer symmetric when comparing the x_1 and x_2 directions. Initially, $a_{11} > a_{22}$, indicating that current is stronger when moving in the x_1 direction, parallel to the particles, than when moving in the x_2 direction, orthogonal to the particles. However, as λ becomes large, the difference between the two becomes negligible.

The off-diagonal entries show a more interesting pattern. For all values of λ, a_{21} is larger than a_{12} in absolute value. a_{12} tends to 0 very quickly, but a_{21} does not follow a consistent pattern. Eventually, it becomes small, but remains much larger than a_{12}. This makes sense intuitively; we would expect a more significant loss of current when moving orthogonal to the particles than when moving parallel to them.

Particles Arranged in a Spiral

In this next case, the four particles will be arranged in a zig-zag pattern. This is meant to be a two-dimensional analog of particles arranged in a helix inside a unit cube in three dimensions. As such, we will refer to this arrangement as a spiral. The setup is shown in Figure 6.

The values of the matrix A for the different values of λ are shown in Table 3. Even though this arrangement is not symmetric, A is close to a symmetric matrix for all values of λ. The values of the main diagonal entries are similar to those in the previous two cases, indicating a similar increase in current. The off-diagonal entries still decrease, but not as rapidly. We thus see a more significant loss of current in this case, particularly while current is flowing in



(a) Approximation of ψ (b) Approximation of χ

Figure 6: Solutions for ψ and χ for the particles arranged in a spiral pattern. The Debye length is $\lambda = 0.1$

λ	0.1	0.316	1	3.16	10
a_{11}	2.532	5.646	8.124	8.673	8.736
a_{12}	0.0202	0.1944	0.0825	0.0108	0.0011
a_{21}	0.1911	0.2356	0.0602	0.0071	7.22E-4
a_{22}	2.702	5.687	8.101	8.669	8.736

Table 3: Entries of Matrix A for the particles arranged in a zig-zag pattern, using different values of λ.

the x_1 direction. This makes intuitive sense, as the particles are arranged in vertical columns.

Conclusion and Future Research

In this project, we see how homogenization can be applied to physical problems. We defined conductivity in a square material based on the work-function mismatch between two materials. The result was a PDE system which was difficult to solve, and reduced it to a simpler problem on the macroscale with constant coefficients instead of variable ones. This allowed us to observe how material properties, in particular particle structure, affected the conductivity as current flowed through in different directions.

Regarding conduction, we find that the three arrangements of particles we studied – the diagonal, horizontal, and spiral arrangements– were similar to each other in effective conductivity. If the Debye length λ is small, then the particles do little to enhance the conductivity of the material. If λ is large, then conductivity is enhanced strongly throughout the entire material, and the arrangement of the particles makes very little difference. When λ takes values that are neither too small nor too large, the particle arrangement does have an effect on how conductivity is enhanced when comparing horizontal and vertical current flow. In the diagonal case, this difference was small, which is to be expected since this arrangement is fairly symmetric. The spiral case was still fairly symmetric. The only case where there was any meaningful difference was in the horizontal case. In this arrangement, conductivity was enhanced more strongly when current flow was horizontal than when it was veritcal. In all three cases, the off-diagonal entries of A were small, and fairly negligible in the diagonal case. In the horizontal and spiral cases the off-diagonal entries, while still small, were large enough to imply a meaningful loss of conductivity for current flow in any direction. Of the three arrangements, the diagonal case was the most consistent due to its symmetry.

A future project could consider this problem in three dimensions instead of just two. This would allow for a greater variety of particle arrangements to analyze. The matrix A would also have more off-diagonal entries, which coud lead to a more meaningful insight into what these values really represent, especially if they are not all similar to each other.

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