A problem of optimal design of composites

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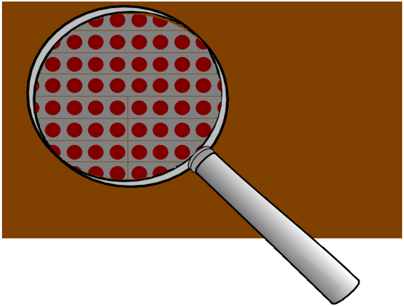
Oct. 25th, 2007

Composite materials

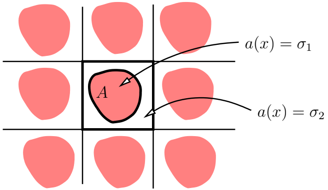


Composites are engineered materials made from two or more constituent materials with significantly different physical properties (For ex. Thermal conductivity).
The mixing of the materials is at a small scale, we compute the conductivity properties at a larger scale by a process called homogenization.

Periodic composites

In a periodic two-component composite, the conductivity at each point is given by a periodic function a with the following form in the unit cube Q.

$$a(x) = \begin{cases} \sigma_1 & \text{if } x \in A \\ \sigma_2 & \text{if } x \in Q \setminus A \end{cases}$$



Where A is the part of the cube covered by the first constituent material.

homogenization

If the function a is periodic in cubes of size ε, we have equations like

$$\operatorname{div}(a(x/\varepsilon)\nabla u^\varepsilon(x)) = f(x)$$

As $\varepsilon \to 0$, the solutions u^ε will converge to a solution u to the *homogenized* problem:

$$\operatorname{div}(A_{\text{eff}}\nabla u(x)) = f(x)$$

where the matrix A_{eff} depends on σ_1, σ_2 and the exact shape of the set A.

Cell problem

Formula to obtain A_{eff}

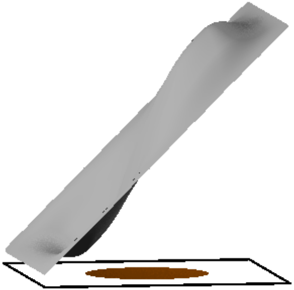
The matrix A_{eff} is a self-adjoint matrix such that

$$\langle A_{\text{eff}}\, v, v\rangle = \min_{w \in H^1_{\text{per}}(Q)} \int_Q a(x)|v + \nabla w|^2 \, \mathrm{d}x.$$

Note that $\langle A_{\text{eff}}\, v, v\rangle$ is the energy of a function $u(x) = x \cdot v + w(x)$ that is periodic perturbation of a plane and solves

$$\operatorname{div}(a(x)\nabla u) = 0 \qquad \text{in } Q$$

Interpretation of the cell problem



The function $u = x \cdot v + w$ is a periodic perturbation of a plane that solves $\mathrm{div}(a(x)\nabla u) = 0$ in Q.

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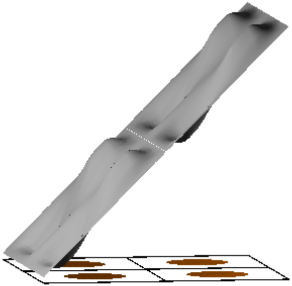

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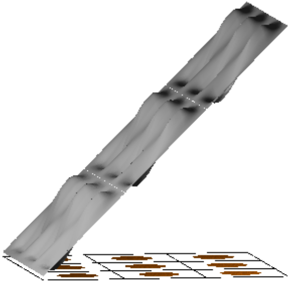

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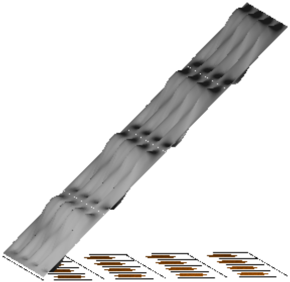

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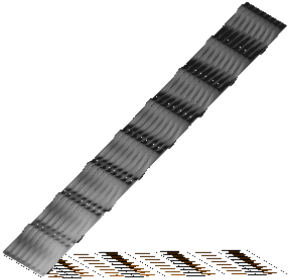

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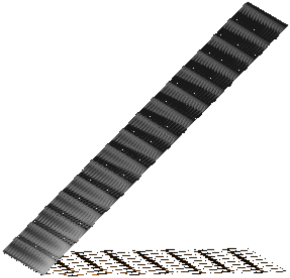

In a coarser scale, the function u approximates a plane. Its energy is still $\langle A_{\text{eff}} v, v \rangle$.

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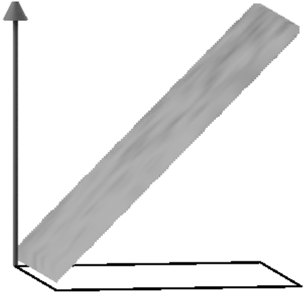

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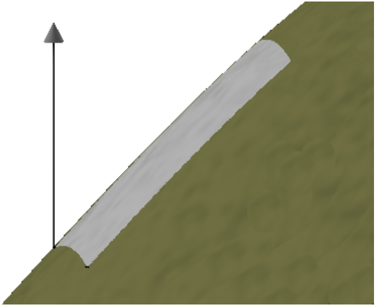

In an even larger scale, it could be a piece of a smooth function.

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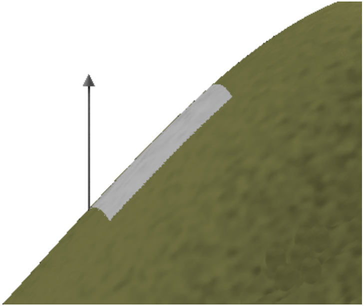

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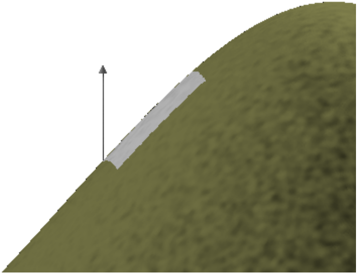

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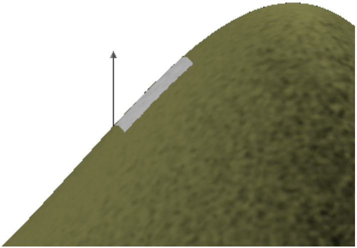

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Effective conductivity.

In general A_{eff} is a selfadjoint $n \times n$ matrix.

In case the set A (the part of the unit cube occupied by the first component) is cubically symmetric, then we know A_{eff} will be a scalar $a_{\text{eff}} I$.

First Question of optimization.

Question

Given $\sigma_1 < \sigma_2$ and $\mu > 0$, what is the maximum value that a_{eff} can take for all cubically symmetric shapes A such that $|A| = \mu$??

Answer

The maximum conductivity is given by the Hashin-Shtrikman bound:

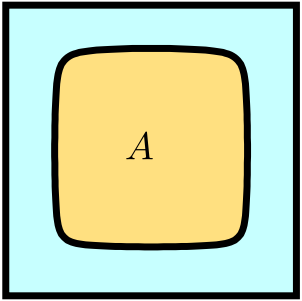
$$a_{\text{eff}} \leq \mu\sigma_1 + (1-\mu)\sigma_2 - \frac{\mu(1-\mu)(\sigma_2-\sigma_1)^2}{(n\sigma_2 + (1-\mu)(\sigma_1-\sigma_2))}$$

Moreover, there is a unique connected shape A that realizes the bound and it is given by the contact set of an obstacle problem.

General Vigdergauz structures

The unique connected shape A that achieves the Hashin-Shtrikman bound is the contact set of the following *obstacle* problem.

- q is a Q-periodic function.
- $q \geq -|x|^2$ in Q.
- $\triangle q(x) = k$ for every x where $q(x) > -|x|^2$.
- $\triangle q(x) \leq k$ in Q.



Liu, James and Leo - 2006

A more symmetric problem

Consider a composite where one constituent is a good thermal conductor (conductivity 1) but a bad electric conductor (conductivity ε). The other has the exact oposite properties: thermal conductivity ε and electric conductivity 1.

Let a_{eff} and b_{eff} be the effective thermal and electric conductivities of the mix.

In a series of papers, Torquato, Hyun and Donev studied the problem of maximizing $a_{\text{eff}} + b_{\text{eff}}$ from all cubically symmetric shapes A in 3D such that $|A| = |Q|/2$.
Not that if we exchange A with $Q \setminus A$, the quantity $a_{\text{eff}} + b_{\text{eff}}$ does not change.

Bergman's bounds

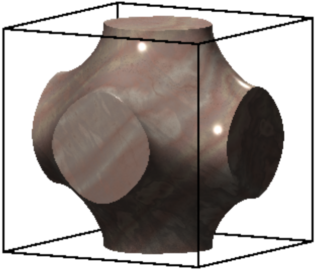
Using classical cross-property bounds due to Bergman (1978), we can obtain the following upper bound in 3D:

$$a_{\text{eff}} + b_{\text{eff}} \leq (1+\varepsilon) - \frac{(1-\varepsilon)^2}{3(1+\varepsilon)}.$$

Question: Is the bound achievable?

Pseudo-answer: Numeric computations by Torquato, Hyun and Donev suggest it is.

The expected optimal microstructure



The expected shape of an optimal structure A would be triply connected.

Moreover $Q \setminus A$ would be triply connected too.

Moreover A and $Q \setminus A$ should be congruent sets due to the symmetry of the problem.

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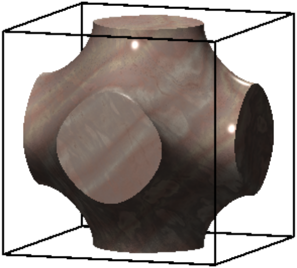

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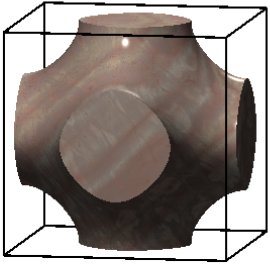

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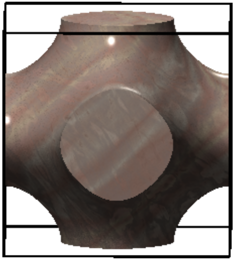

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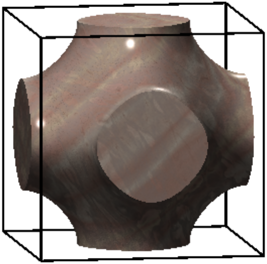

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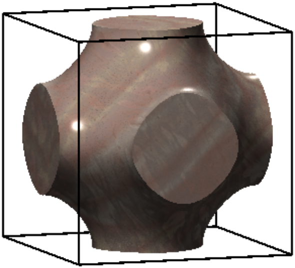

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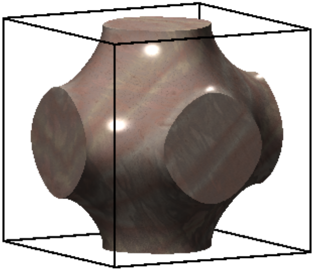

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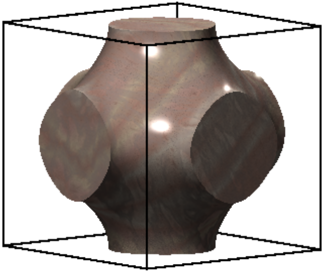

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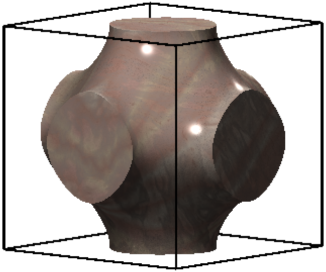

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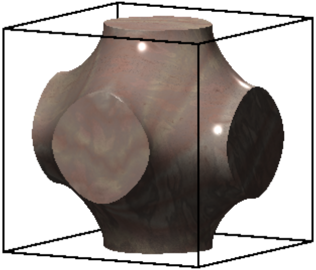

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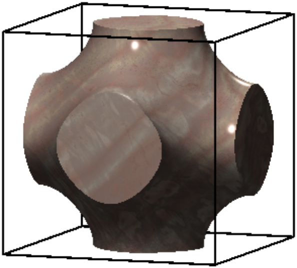

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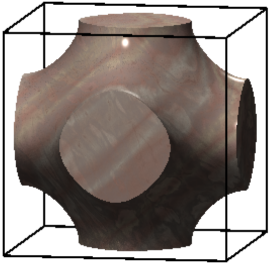

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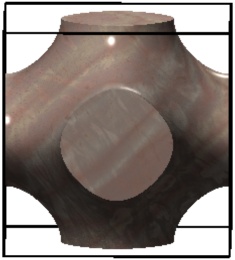

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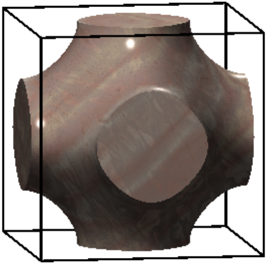

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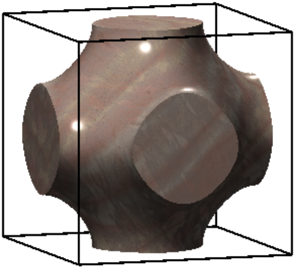

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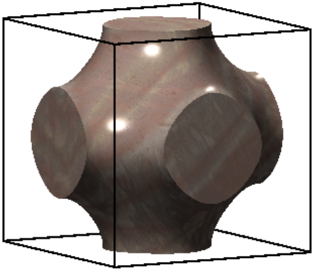

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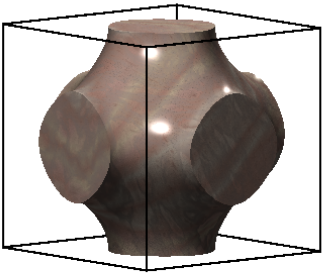

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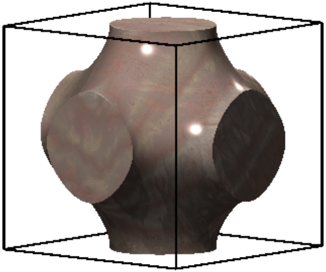

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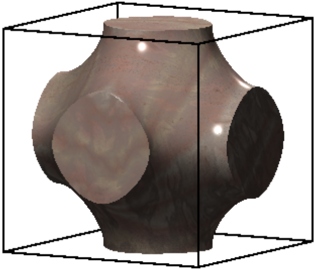

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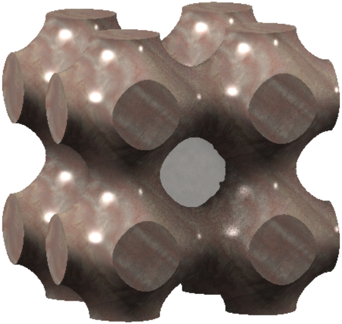

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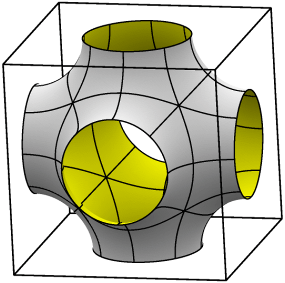
Conjecture.

From the numeric computations it was natural to believe that ∂A was the Schwartz P surface.

The Schwartz P surface is a bicontinuous periodical minimal surface.



Picture of the Schwartz P surface from the website of Ken Brakke.

Characterization of optimal structures

Theorem

Bergman's upper bound is achieved for a set $A \subset Q$ if and only if the periodic solution to

$$\triangle q = \begin{cases} 1 & \text{in } A \\ -1 & \text{in } Q \setminus A \end{cases}$$

satisfies

$$D^2 q(x) = \begin{cases} M(x) + \nu \otimes \nu & \text{on the } A \text{ side of } \partial A \\ M(x) - \nu \otimes \nu & \text{on the } Q \setminus A \text{ side of } \partial A \end{cases}$$

for some matrix M such that $M(x) \cdot \nu = 0$.

Proof in the blackboard.

Counterproof of the conjecture

Question

Can Bergman's upper bound be achieved if ∂A has mean curvature zero?

If that was the case, it can be shown that

- q is constant $(= 0)$ on ∂A.
- q_ν is also constant on ∂A.

So, at the same time we would have that q^+ and q^- solve the one phase problem, and q solves the two-phase membrane problem.

For a given set A, these conditions can be checked numerically in a very simple way. Indeed, they are **not** satisfied if ∂A is the Schwartz P surface.