On the effective properties of heterogeneous materials

Carmen Calvo Jurado

"Applied Mathematics" **Research Group**

Department of Mathematics
University of Extremadura

First Joint Meeting Évora-Extremadura on Mathematics

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Research lines

- Lie Algebras: Generalization and applications
- Fourier Analysis
- Computational methods in Applied Mathematics
- Homogenization. Micromechanics. Composite materials

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Homogenization

Homogenization of partial differential equations in random perforated domains

Bounds

Effective conductive properties of transversely isotropic two-phase composites

Research lines

- Lie Algebras: Generalization and applications
- Fourier Analysis
- Computational methods in Applied Mathematics
- Homogenization. Micromechanics. Composite materials

Carmen Calvo-Jurado, Juan Casado-Díaz, Manuel Luna Laynez

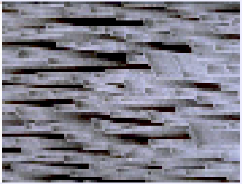
Homogenization of nonlinear Dirichlet problems in random perforated domains *Nonlinear Analysis*, 133 250-274, 2016.

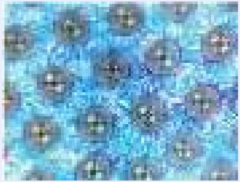
Carmen Calvo-Jurado, William J. Parnell

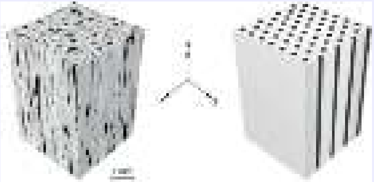
Hashin Shtrikman bounds on the effective thermal conductivity of a transversely isotropic two phase composite material *J. Math. Chem.*, 53 828-843, 2015.

Introduction
Fibre-Reinforced Materials (FRMs)

- FRMs used extensively as composites
- Superconducting, insulation, aircraft, tissue engineering applications,...
- FRMs appear "naturally", e.g. in bone and soft tissue





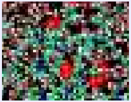


Introduction
Two-phase materials

Two-phase composites

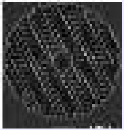
- Tissue engineering applications
- Laser-induced thermal effects: therapeutic and diagnostic applications

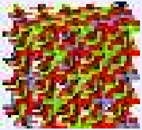
Introduction
Motivation



"Material Sciences"

Composites, crystals, polymers, perforated domains...





Physical parameters

Elasticity, conductivity, deformation, displacement,...

very large number of heterogeneities

Computational methods are difficult to implement

Effective properties

Homogenization Theory

(Sánchez-Palencia, Murat, Tartar, Lurie, Cherkaev,...)

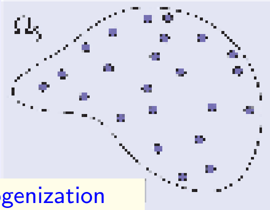
Bounds

(Voigt-Reuss, Hashin-Shtrikman,...)

Introduction
General theory of Homogenization

$$A^\delta u^\delta = f \text{ in } \mathcal{O}_\delta$$

u^δ: conductivity, displacement,...



Homogenization

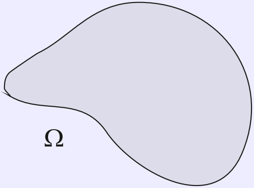
Asymptotic behavior

$\delta \to 0$

Homogenizated problem

$$A^* u^* = f \text{ in } \Omega$$

Overall, effective, behavior of the model



Homogenization of the Poisson equation with Dirichlet conditions in random perforated domains

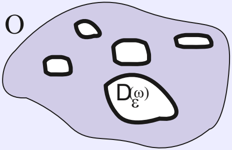
Carmen Calvo Jurado[1] Juan Casado Díaz[2]
Manuel Luna Laynez[2]

[1] University of Extremadura
[2] University of Sevilla

- $(\Omega, \mathcal{F}, P)$ a probability space.
- $\mathcal{O} \subset \mathbb{R}^N$ a bounded open set.
- $\mathcal{D}_\varepsilon(\omega) \subset \mathcal{O}$, a family of closed subsets ("holes") where we assume a Dirichlet boundary condition.

Homogenization

$$\begin{cases} -\Delta u_\varepsilon = f_\varepsilon(x, \omega) & \text{in } \mathcal{O}_\varepsilon(\omega) \\ u_\varepsilon = 0 & \partial\mathcal{O}_\varepsilon(\omega), \quad P\text{-a.e. } \omega \in \Omega. \end{cases}$$



The random homogenization problem

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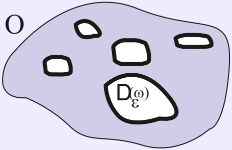

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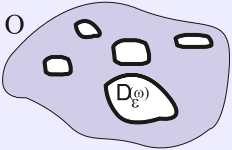

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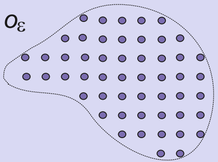
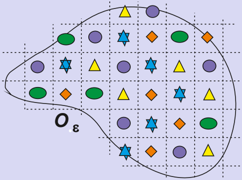
- $\mathcal{O}_\varepsilon(\omega) = \mathcal{O} \setminus D_\varepsilon(\omega), \quad P\text{-a.e. } \omega \in \Omega.$

Preliminaries: Periodic problem

Small balls periodically distributed in $\mathbb{R}^N$

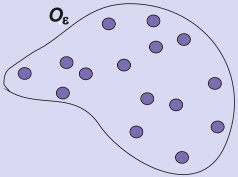


Non-spherical holes periodically distributed in $\mathbb{R}^N$

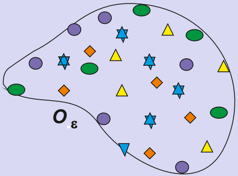


Preliminaries: Periodic problem

Spherical holes distributed in $\mathbb{R}^N$



Non-spherical holes periodically distributed in $\mathbb{R}^N$



Hypotheses on the holes

- $\forall x \in \mathbb{R}^N$, $T(x) : \Omega \to \Omega$, an ergodic N-dynamical system preserving the measure in Ω:

(H1) There exists $\tilde{\Omega} \subset \Omega$, $(\tilde{\Omega}, \tilde{\mathcal{F}})$ and $\delta \in (0,1)$ such that for every $\omega \in \Omega$, we have

$$\mathrm{card}\Big(\{z \in B(0,2\delta) : \ T(z)\omega \in \tilde{\Omega}\}\Big) \leq 1.$$

(H2) For every $\tilde{\omega} \in \tilde{\Omega}$, there exists a closed sets family $R_{\tilde{\omega}}$, in $\mathbb{R}^N$, such that

$$\mathrm{diam}(R_{\tilde{\omega}}) \leq C, \qquad \text{with } C > 0.$$

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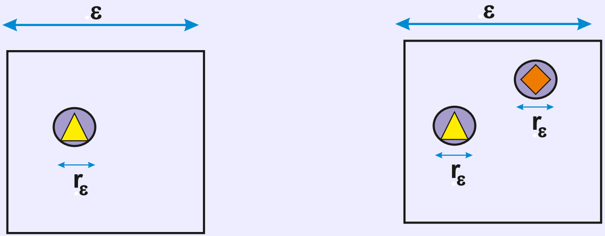
☞ Note that (H1) guarantees that neighboring holes are sufficiently separated.

Hypotheses on the holes

$$\mathcal{O}_\varepsilon(\omega) = \mathcal{O} \setminus D_\varepsilon(\omega)$$

$$D_\varepsilon(\omega) = \bigcup_{T(z)\omega\in\tilde{\Omega}} \left(\varepsilon z + \underbrace{\varepsilon^{\frac{N}{N-2}} R_{T(z)\omega}}_{r_\varepsilon}\right)$$



Main Result

Main Result

There exists a function $\zeta \in L^\infty(\mathcal{O})$ such that for a.e. $\omega \in \Omega$, the solution of

$$\begin{cases} -\Delta u_\varepsilon(x,\omega) = f_\varepsilon(x,\omega) & \text{in } \mathcal{O}_\varepsilon(\omega), \\ u_\varepsilon(x,\omega) = 0 & \text{on } \partial\mathcal{O}_\varepsilon(\omega), \end{cases} \quad P\text{-a.e. } \omega \in \Omega$$

converges weakly in $L^2_P(\Omega; H^1_0(\mathcal{O}))$ to the unique solution u of

$$\begin{cases} u \in L^2(\Omega; H^1_0(\mathcal{O})) \\ -\Delta u + \zeta(x) u = f \text{ in } \mathbb{R}^N. \end{cases}$$

▷ The term $\zeta\, u$ is similar to the "strange term" which appear in the periodic case.

▷ The term ζ does not depend on ω. Thus, if we take f independent of ω, the limit problem is *deterministic*.

On the effective thermal conductivity for a transversely isotropic two phase composite material

Carmen Calvo Jurado[1] William J. Parnell[2]

[1] University of Extremadura
[2] University of Manchester

Preliminaries: Prediction physical properties of composites

Maxwell (1873), Rayleigh (1892), Einstein (1905),...

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Prediction physical properties of composites

Maxwell (1873), Rayleigh (1892), Einstein (1905),...

Voigt (1889), Reuss (1929), Hill (1951)

Only information about volume fraction is incorporated

$$K_{ij}^R \leq K_{ij}^* \leq K_{ij}^V$$

$$(K^R)_{ij}^{-1} = \sum_{r=0}^{n} \phi_r (K^r)_{ij}^{-1}, \qquad K_{ij}^V = \sum_{r=0}^{n} \phi_r K_{ij}^r.$$

Independent of any characteristic of the symmetry of the microstructure

Too wide to be of predictive interest

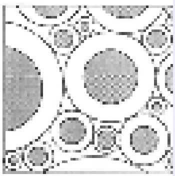
Preliminaries:
Prediction physical properties of composites

Maxwell (1873), Rayleigh (1892), Einstein (1905),...

Hashin-Shtrikman bounds (1966)

Without information about the distribution of the phases

Optimal: we can find geometries such that they are attained



Basic formulation

- $\Omega \subset \mathbb{R}^N$
- $\delta, \varepsilon > 0$
- Two phases $\Omega^0(\delta, \varepsilon), \Omega^1(\delta, \varepsilon) \subset \Omega$
  - $\Omega^0(\delta, \varepsilon) \cup \Omega^1(\delta, \varepsilon) = \Omega$
  - $\Omega^0(\delta, \varepsilon) \cap \Omega^1(\delta, \varepsilon) = \emptyset$

$$-div\,(\mathbf{K}(x)\nabla T) = f \quad \text{in } \Omega$$

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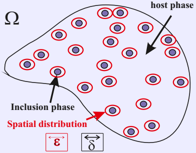

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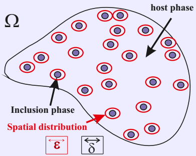

$f \in H^{-1}(\Omega)$ the internal source term

Basic formulation

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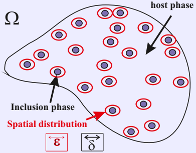


Notation: Macroscopic effective properties

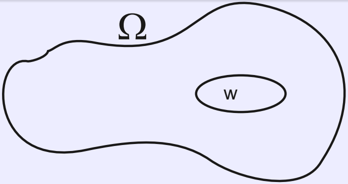
$$\mathbf{K}^*$$

The single inclusion problem

Assuming an ellipsoidal single inclusion $\omega \in \Omega$, one has uniformity of thermal gradients inside it given uniform temperature gradients in the far field

- Eshelby (1961): **The** ***weak*** **conjecture.** [Milton, Kohn, Liu, (2008)]

  Given some inclusion $\omega \in \Omega$, if the strain induced inside the inclusion is uniform *for any homogeneous boundary condition*, then the inclusion must be an ellipsoid.



☞ Ellipsoidal inclusions play a central role in the theory of composites

Hashin-Shtrikman (1963)

- Effective energy:

$$W^*(\bar{\mathbf{e}}) = \inf_{\mathbf{e}\in\mathcal{E}} \int_\Omega \mathbf{W}(x,\mathbf{e})\,d\mathbf{x} = \frac{1}{2}\bar{\mathbf{e}}\cdot\mathbf{K}^*\bar{\mathbf{e}}.$$

$$\mathcal{E} = \{\mathbf{e} : \text{ there exists } T \in H^1(\Omega) \text{ such that } \mathbf{e} = \nabla T,\ T = \bar{T} \text{ on } \partial\Omega\}.$$

- Homogeneous comparison material:

$$\mathbf{K}^c$$

Main result

Theorem

Under the hypotheses above,

$$\mathbf{W}^*(\bar{\mathbf{e}}) \geq (\leq) \frac{1}{2}\bar{\mathbf{e}} \cdot \mathbf{K}^c \bar{\mathbf{e}} + \frac{1}{2}\bar{\mathbf{e}} \cdot \bar{\boldsymbol{\tau}}^*$$

whenever that $\mathbf{K}^c \leq \min_{0\leq r\leq n} \mathbf{K}^r (\geq \max_{0\leq r\leq n} \mathbf{K}^r)$, where

$$\bar{\boldsymbol{\tau}}^* = \sum_{k=0}^{n} \phi_k \boldsymbol{\tau}_k^*$$

is the average of the *optimal polarizations* $\boldsymbol{\tau}_k^*$, which satisfy the relations

$$\begin{cases} (\mathbf{K}^0 - \mathbf{K}^c)^{-1}\boldsymbol{\tau}_0^* - \dfrac{1}{\phi_0}\displaystyle\sum_{k=1}^{n}\sum_{\ell=1}^{n} \mathbf{M}^{(k\ell)}(\boldsymbol{\tau}_\ell^* - \boldsymbol{\tau}_0^*) = \bar{\mathbf{e}} \\ (\mathbf{K}^k - \mathbf{K}^c)^{-1}\boldsymbol{\tau}_k^* + \dfrac{1}{\phi_k}\displaystyle\sum_{\ell=1}^{n} \mathbf{M}^{(k\ell)}(\boldsymbol{\tau}_\ell^* - \boldsymbol{\tau}_0^*) = \bar{\mathbf{e}}, \quad k = 1, \ldots, n. \end{cases}$$

where $\overline{\mathbf{M}}^{(k\ell)} = \phi_\ell(\mathbf{P}_s^k - \phi_k \mathbf{P}_d^{(k\ell)}), \quad k, \ell = 1, \ldots, n.$

Main result

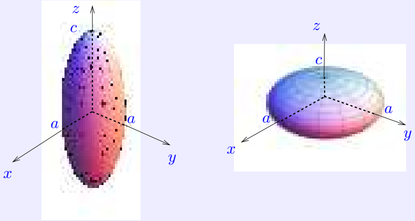
$$\overline{\mathbf{M}}^{(k\ell)} = \phi_\ell({\mathbf{P}_s}^k - \phi_k {\mathbf{P}_d}^{(k\ell)}), \quad k, \ell = 1, \ldots, n.$$

- $\mathbf{P}_s^k$: shape-Hill tensor associated with the kth-phase inclusion Ω_k (δ)
- $\mathbf{P}_d^{k\ell}$: distribution-Hill tensor computed over an ellipsoid $\Omega_d^{k\ell}$ associated with the distribution between the $k\ell$-phases inclusions (ε)

THE HILL P-TENSOR
SPHEROIDAL TI INCLUSIONS IN A TI HOST PHASE

Oblate or prolate spheroidal TI inclusions with semi-axes $a = a_1 = a_2 \neq a_3$ inside an also TI matrix material, where the a_3 axis is aligned along x_3 the axis of transverse isotropy of the host

Transversely isotropic (TI) FRMs



Aspect ratio: $\rho = c/a$

- $\rho > 1$ (prolate)
- $\rho < 1$ (oblate)

Example: Spheroidal distribution has different shape to that of the inclusion shape $\mathbf{P}_s \neq \mathbf{P}_d$

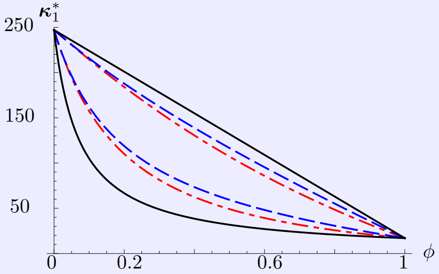
Kovar inclusions in aluminum host phase

- Aluminum: $\kappa_1^0 = 247$ W/Km (CTE$= 23\ 10^{-6}/^oC$)
- Kovar: $\kappa_1^1 = 17$ W/Km (CTE$= 5.1\ 10^{-6}/^oC$)

κ_1^*

Example: Spheroidal distribution has different shape to that of the inclusion shape $\mathbf{P}_s \neq \mathbf{P}_d$

- $\rho_s = 1$: spherical inclusions distributed with spheroidal oblate symmetry $\rho_d = \sqrt{\phi}$. (— · — · — ·)
- $\rho_s = 1$: spherical inclusions distributed with spheroidal prolate symmetry $\rho_d = \frac{1}{\phi}$. (— — — —)
- Voigt-Reuss bounds (▬▬▬)



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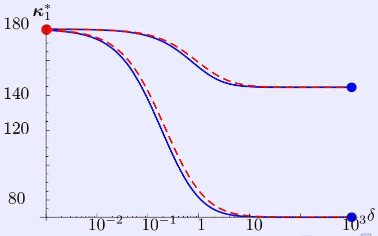
Influence of the spheroidal inclusions

- $\phi = 0.3$: fix volume fraction of kovar inclusion phase
- $\rho_s = \delta$: spheroidal inclusion
- $\rho_d = \varepsilon$: spheroidal distribution with aspect ratios
  - $\rho_d = \varepsilon = \delta\sqrt{\phi} \leq \delta$ (solid blue line)
  - $\rho_d = \varepsilon = \delta$ (dashed red line)
- Limiting cases $\delta \to 0$ (layered) $\delta \to \infty$ (long fibre)



Conclusions

Future work

Conclusions and future work

- Homogenization of random reticulated structures. Conductive and elastic settings
- Theory can be extended to nonlinear multiphase setting (also to elasticity by bounding strain energy)

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Thank you very much

for your attention.