

Composite Properties and Microstructure I: Effective Properties

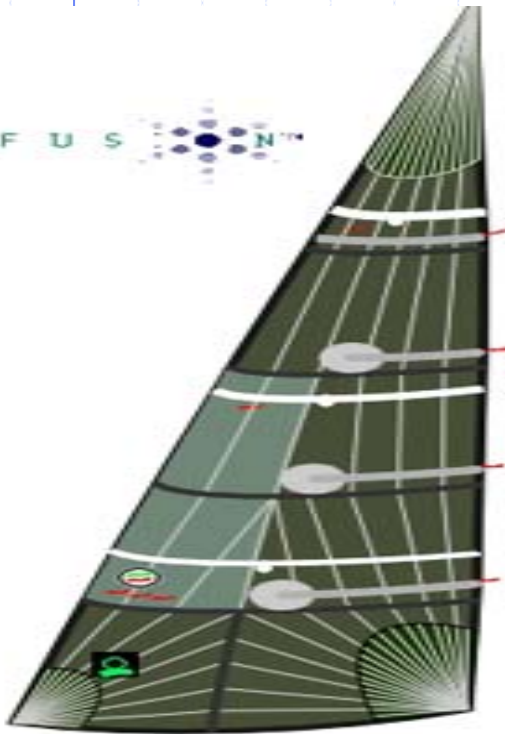
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Composites: Where Mathematics Meets
Industry

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IMA-Institute for Mathematics and its
Applications

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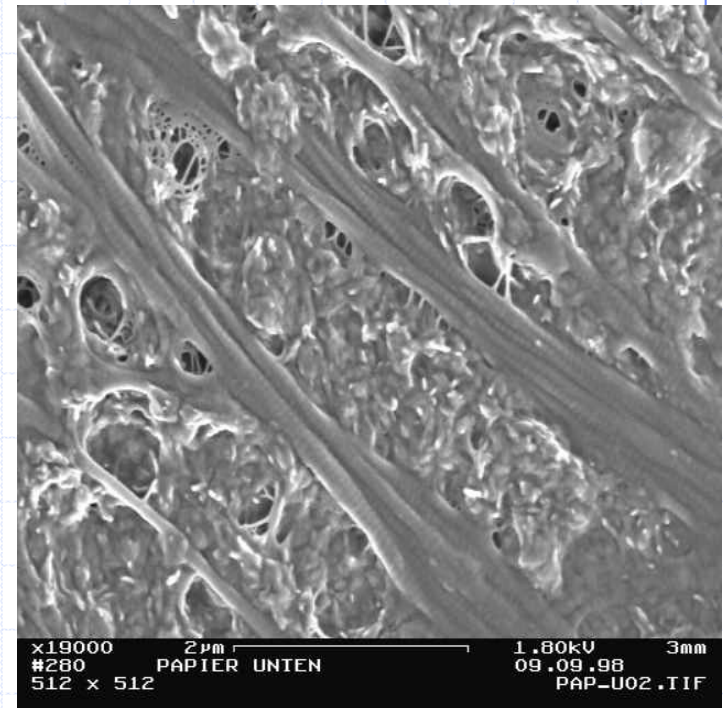
Composite structures



Racing Sail



Fiber reinforced epoxy
Horizontal Stabilizer
Boeing 777

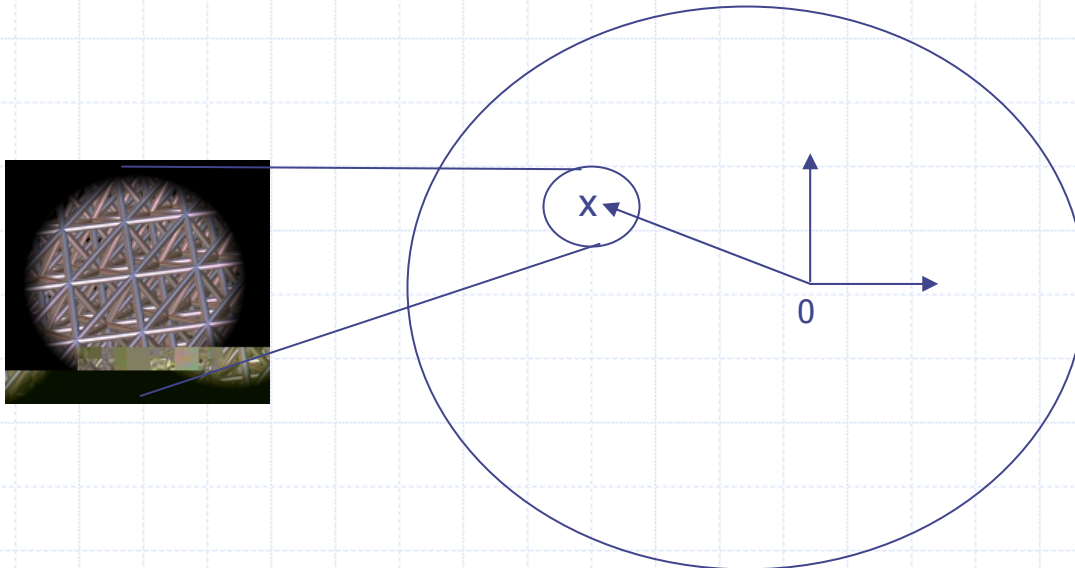


Bone

Multi-scale problem statement

It is supposed that the length scale of the composite microstructure is significantly smaller than the length scale of the load.

The goal is to characterize the behavior of the composite structure when the characteristic length scale of the loading is much larger than the composite microstructure.



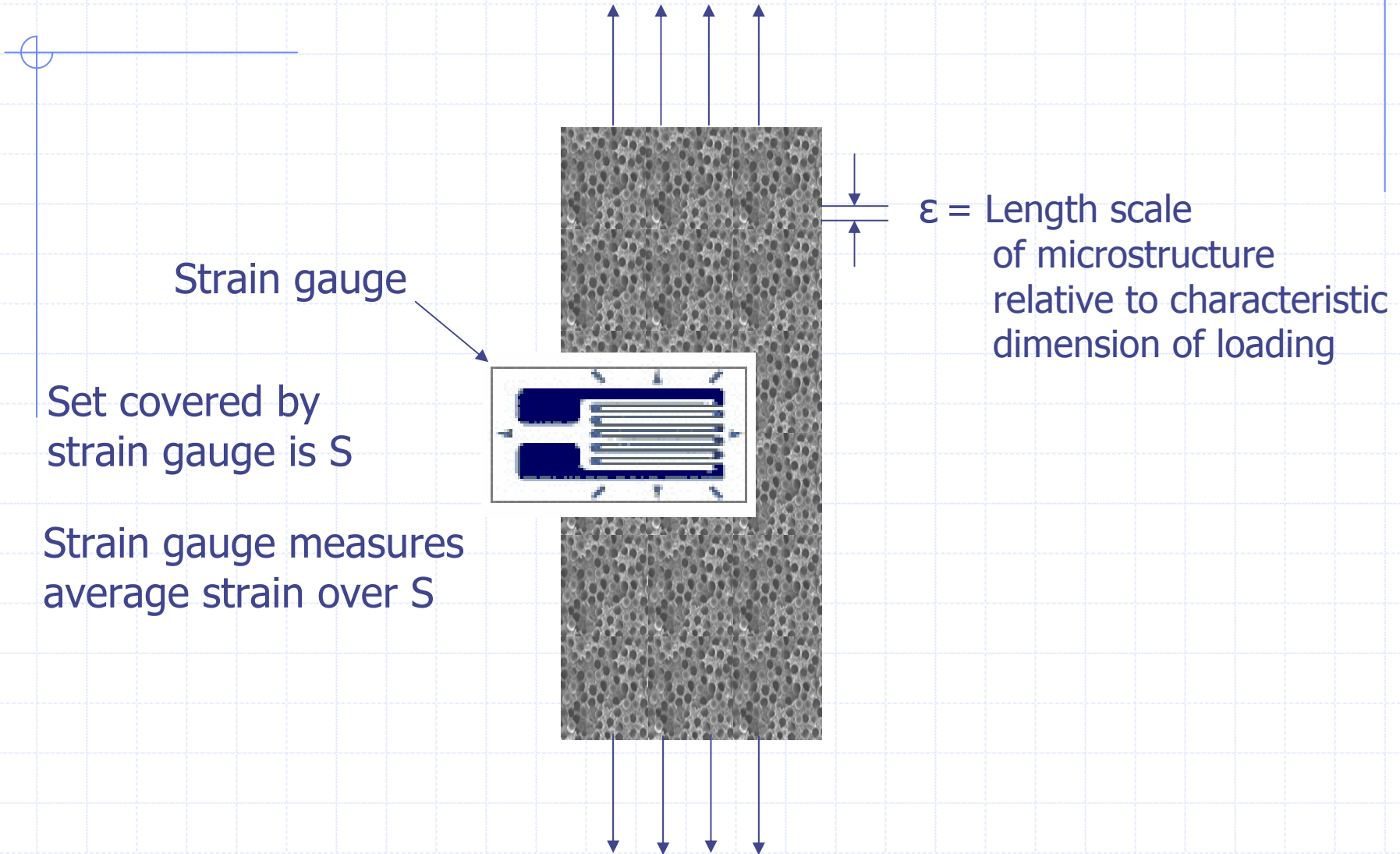


Effective properties such as:

- 1) Effective stiffness
- 2) Effective thermal conductivity
- 3) Effective dielectric constant

Are introduced within the context of homogenization theory.

Homogenization theory provides a way to calculate average strain measured by a strain gauge in microstructured media.



Strain gauge

$\epsilon =$ Length scale of microstructure relative to characteristic dimension of loading

Set covered by strain gauge is S

Strain gauge measures average strain over S

Boundary value problem in periodically microstructured elastic media

Length scale of microstructure $0 < \varepsilon \ll 1$

Elastic displacement field $u^\varepsilon(x)$

Strain tensor $\varepsilon^\varepsilon(x)$ $\varepsilon^\varepsilon = (u_{i,j}^\varepsilon + u_{j,i}^\varepsilon) / 2$

Stress tensor $\sigma^\varepsilon(x)$

Local elastic tensor $C^\varepsilon(x) = C^i$

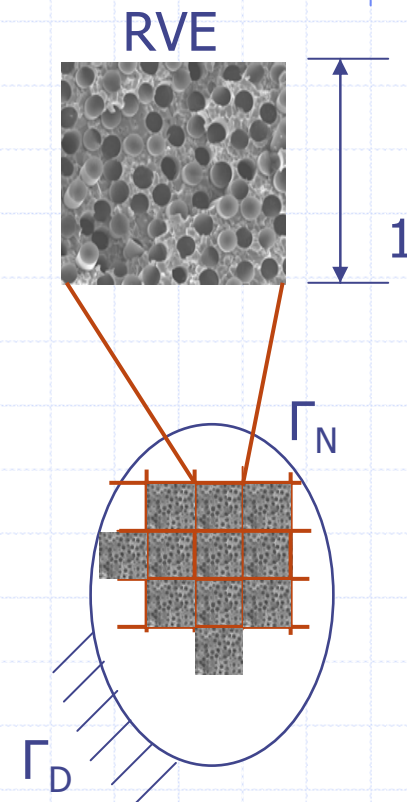
C^i is the elasticity of i^{th} material

Constitutive relation $\sigma^\varepsilon(x) = C^\varepsilon(x)\varepsilon^\varepsilon(x)$

Equation of elastic equilibrium $-\text{div}(\sigma^\varepsilon) = f$

Boundary conditions:

Traction BC on Γ_N $n \bullet \sigma^\varepsilon(x) = g$
 and displacement BC on Γ_D $u^\varepsilon = U$



Homogenization theory; convergence of averages

For any subset S :

$$\frac{1}{|S|} \int_S u^\varepsilon(x) dx \rightarrow \frac{1}{|S|} \int_S u^M(x) dx$$

Average strain over S : $\frac{1}{|S|} \int_S \varepsilon^\varepsilon(x) dx \rightarrow \frac{1}{|S|} \int_S \varepsilon^M(x) dx =$ Average of homogenized strain

$$\frac{1}{|S|} \int_S \sigma^\varepsilon(x) dx \rightarrow \frac{1}{|S|} \int_S \sigma^M(x) dx$$

Homogenized constitutive relation

$$\sigma^M(x) = C^E \varepsilon^M(x)$$

$$\varepsilon^M = (u_{i,j}^M + u_{j,i}^M) / 2$$

Homogenized boundary value problem

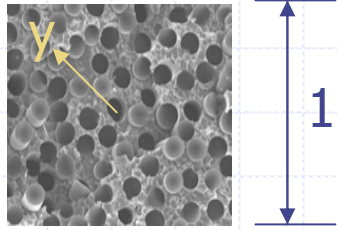
$$- \operatorname{div} \sigma^M = f$$

Traction BC on Γ_N
and displacement BC on Γ_D

$$u^M = U$$

$$n \bullet \sigma^M(x) = g$$

RVE:



Formula for C^E

- ◆ Load unit RVE with homogeneous strain $\bar{\varepsilon}$
- ◆ Local elastic tensor in microstructure = $C(y)$
- ◆ Micro-problem in RVE is to solve for periodic strain fluctuation
- ◆ Local periodic strain fluctuation $e(y)$ solution of:

$$\text{div} (C(y)(e(y) + \bar{\varepsilon})) = 0, \quad \int_Q e(y) dy = 0$$

- ◆ C^E given by:

$$C^E \bar{\varepsilon} = \int_Q C(y)(e(y) + \bar{\varepsilon}) dy$$

Here: Q denotes the RVE

Physical interpretation of the effective elastic tensor C^E

Local stress inside RVE

$$\sigma(y) = (C(y)(e(y) + \bar{\varepsilon}))$$

Average strain over RVE

$$\int_Q (e(y) + \bar{\varepsilon}) dy = \bar{\varepsilon}$$

Effective elasticity relates average stress to average strain

$$\int_Q \sigma(y) dy = C^E \bar{\varepsilon}$$

Approximate formulas for effective elastic tensors

Given only a partial statistical description of the microstructure the goal is to construct an approximation to the effective tensor

Two well known examples are considered

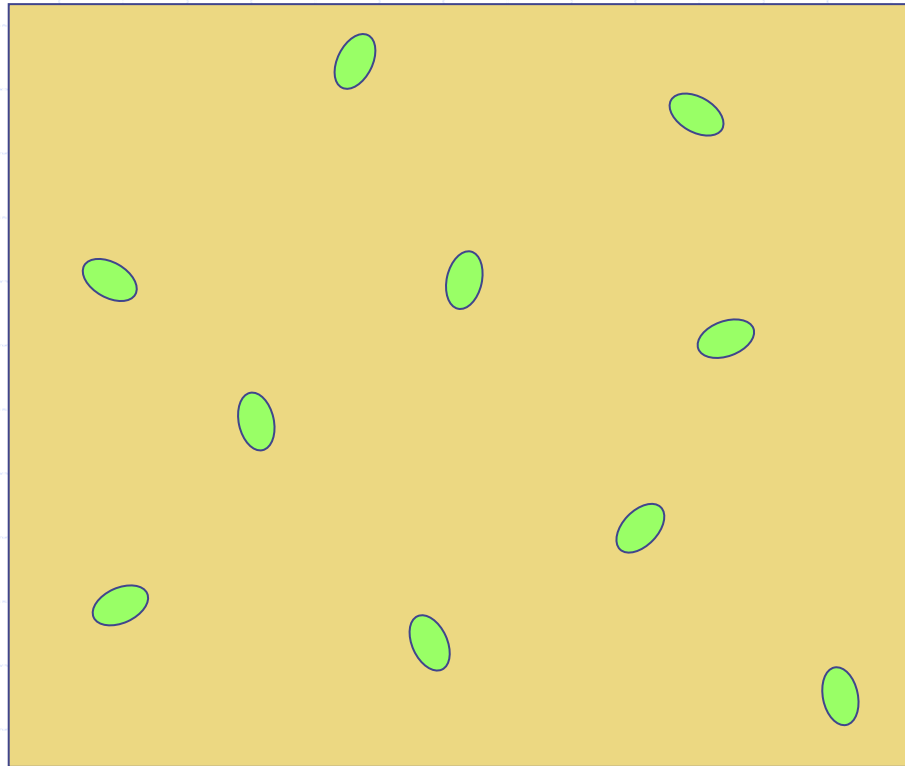
1) Low volume fraction expansions for dilute suspensions.

J.C Maxwell (1873), A. Einstein (1906)

2) Low contrast expansions.

W.F. Brown (1955)

Effective elastic tensor for a dilute suspension of spheroids



Data: C_1 =elastic modulus of spheroids
 C_2 =elastic modulus of matrix,
 θ = volume fraction of spheroids

Expand C^E in a Taylor series with respect to volume fraction

$$C^E = C_2 + \sum_{j=1}^{\infty} B_j \theta^j$$

The coefficients B_j encode geometry of the distribution of the particles in the suspension, eg., they reflect clumping together of the particles, etc.

B_1 is associated with the single particle boundary value problem in an infinite matrix subject to applied field averaged over all orientations

B_2 associated with a two particle boundary value problem in infinite matrix averaged over all two particle configurations

B_j associated with j particle boundary value problem in infinite matrix.

The expansion when only the volume fraction and orientation distribution is known

$$C^E = C_2 + B_1\theta + O(\theta^2)$$

$$B_1 = \langle (C_1 - C_2)\mathbf{T}_1 \rangle$$

Here brackets denote orientation average and \mathbf{T}_1 is the Wu strain tensor and E is the spheroid domain.

The fluctuating part of the strain solves a boundary value problem on the whole space:

$B(R)$ is a Ball of radius R and

$$\mathbf{T}_1 \bar{\varepsilon} = \frac{1}{|E|} \int_E (e^\infty(y) + \bar{\varepsilon}) dy$$

$$\operatorname{div}(C(y)(e^\infty(y) + \bar{\varepsilon})) = 0$$

$$\lim_{R \rightarrow \infty} \frac{1}{|B(R)|} \int_{B(R)} |e^\infty(y)|^2 dy = 0$$

Low volume expansion for spheres

C_1 isotropic and specified by μ_1 κ_1

C_2 isotropic and specified by μ_2 κ_2

Material 1 incompressible: $\mu_1/\kappa_1 = 0$

Material 2 incompressible: $\mu_2/\kappa_2 = 0$


Low volume expansion for the effective shear modulus

$$\mu^E = \mu_2 + \frac{5(\mu_1 - \mu_2)}{2\mu_1 + 3\mu_2} \theta + O(\theta^2)$$

Established rigorously using variational methods by J.B. Keller, L. Rubinfeld, and J. Molyneux (1967)

For rigid spheres $\mu_1/\mu_2 = \infty$ have Einstein's formula (1906)

$$\mu^E = \mu_2 + \frac{5}{2} \theta + O(\theta^2)$$



Formulas for higher order terms in expansion
of elastic tensor see, Chen and Acrivos (1978)

For complete references and detailed derivations
we refer to the recent manuscripts of G. Milton (2002)
and S. Torquato (2002)

Low contrast expansions

Contrast given by $\delta C = C_2 - C_1$

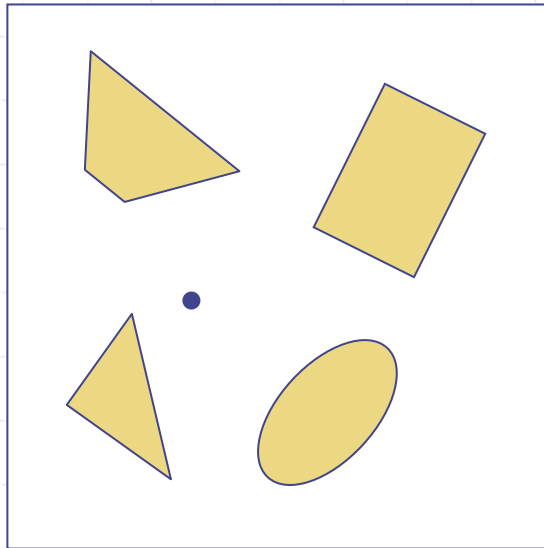
Expand effective elastic tensor in a Taylor Series with respect to contrast
W.F. Brown (1955)

$$C^E = C_2 + \sum_{j=1}^{\infty} A_j (\delta C)^j$$

The geometry is encoded in the coefficients A_j these are given in terms of N-point correlation functions.

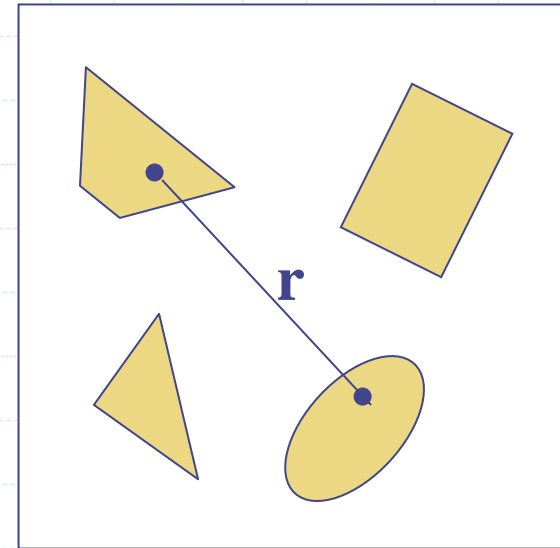
One and two point correlation functions

One point correlation



Probability of a point lying inside the yellow phase
(Volume fraction of the yellow phase)

Two point correlation

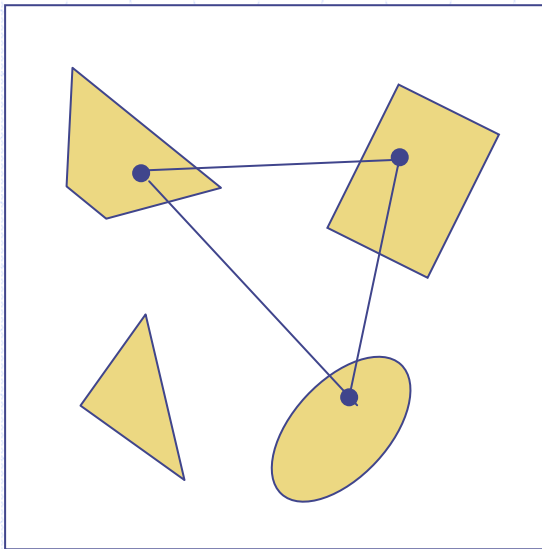


Probability that both ends of a segment lies in yellow phase when thrown into composite randomly

N-point correlation functions

N-point correlation function = probability that N points chosen at random lie inside yellow phase

An example of three point correlation.



Probability that all vertices of a triangle lies in yellow phase when thrown into composite randomly

One, two, and three-point correlation Functions

These statistical functions can be computed using techniques from image analysis. J. Berryman 1988.

Coefficients A_j of contrast expansion

Set $\delta C(y) = C_1 - C_2$, for y in material one

$\delta C(y) = 0$, for y in material two

Set $e^0(y) = \bar{\varepsilon}$

And iterate according to

$$\operatorname{div}(C_2 e^{j+1}(y)) = -\operatorname{div}(\delta C(y) e^j(y)), j = 0, 1, 2, \dots$$

And for $j=1, 2, \dots$ set $A_j \bar{\varepsilon} = \int_Q \delta C(y) e^j(y) dy$

A_j is given in terms of the j -point correlation function
W.F. Brown (1955), M. J. Beran (1965)

An Example: Bulk modulus for isotropic effective elastic tensor

$$\delta\kappa = \kappa_2 - \kappa_1 \qquad \delta\mu = \mu_2 - \mu_1$$

$$\kappa^E = \kappa_2 + \delta\kappa A_1 + (\delta\kappa)^2 A_2 + (\delta\kappa)^3 A_3^1 + \delta\mu (\delta\kappa)^2 A_3^2$$

$$A_1 = \theta$$

G. Milton (1982)

$$A_2 = -\frac{3\theta(1-\theta)}{\theta(3\kappa_1 + 4\mu_1) + (1-\theta)(3\kappa_2 + 4\mu_2)}$$

$$A_3^1 = \frac{9\theta(1-\theta)(1-2\theta)}{[\theta(3\kappa_1 + 4\mu_1) + (1-\theta)(3\kappa_2 + 4\mu_2)]^2}$$

Here ζ_1 is a geometric parameter given in terms of the three point correlation function

$$A_3^2 = \frac{12\theta(1-\theta)(\zeta_1 - \theta)}{[\theta(3\kappa_1 + 4\mu_1) + (1-\theta)(3\kappa_2 + 4\mu_2)]^2}$$

$$0 \leq \zeta_1 \leq 1$$

The parameter ζ_1 is computed for cubic arrays of spheres in McPhedran and Milton (1981)

Extensive references to the literature and detailed analysis can be found in the recent books by G. Milton (2002) and S. Torquato (2002)

Bounds on effective properties: An example from heat conduction inside composite media

Consider the ensemble of composite samples made from two isotropic heat conductors with same volume fractions – having an isotropic effective conductivity $\Sigma^E = \sigma^E \mathbf{I}$.

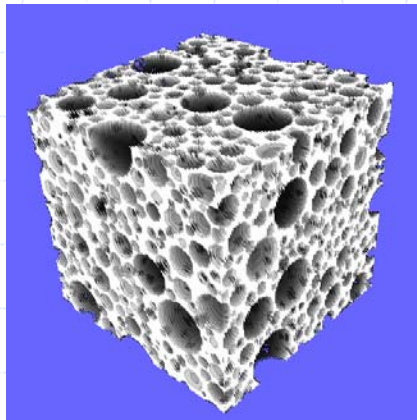
Subject each sample to the same imposed temperature gradient.

Find lower and upper bounds on the effective thermal conductivity σ^E .

Identify realizations that attain the bounds.

Setting

RVE



Cube filled with composite made from two heat conductors. The volume fractions of each is prescribed.

Conductivities: $\sigma_1 > \sigma_2$

Volume fractions: θ_1, θ_2

$\Delta T = 0$ Inside each phase

$n \bullet \sigma_1 \nabla T = n \bullet \sigma_2 \nabla T$ On interface

$\langle \nabla T \rangle = E$ and $T - E \bullet x$ is periodic on the cube

Effective Conductivity

$\sigma(y)$ is the local conductivity
taking the value σ_1 inside material one and σ_2
inside material two.

The effective conductivity is given by

$$\Sigma^e E = \int_Q \sigma(y) \nabla T(y) dy$$

Bounds of Hashin and Shtrikman for effective properties

Hashin Shtrikman bounds on effective conductivity for isotropic composites (1962).

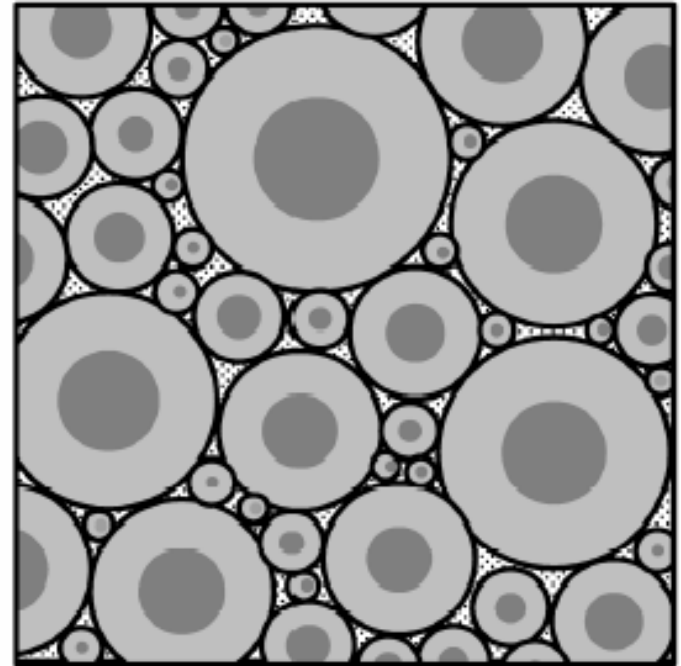
$$\sigma_2 + \frac{3\theta_1\sigma_2(\sigma_1 - \sigma_2)}{3\sigma_2 + \theta_2(\sigma_1 - \sigma_2)} \leq \sigma^e$$

$$\sigma^e \leq \sigma_1 + \frac{3\theta_2\sigma_1(\sigma_2 - \sigma_1)}{3\sigma_1 + \theta_1(\sigma_2 - \sigma_1)}$$

Coated sphere assemblage of Hashin and Shtrikman

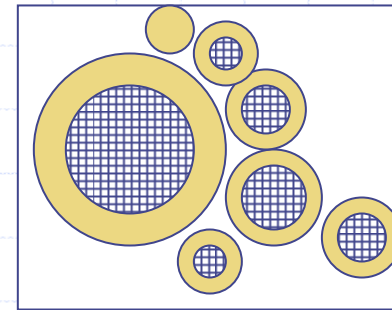
Step I: Fill the RVE with a sphere packing with sphere sizes ranging to the infinitesimal.

Step II: Place a smaller concentric sphere inside each sphere such that the ratio of the radii of the outer and inner spheres is the same.

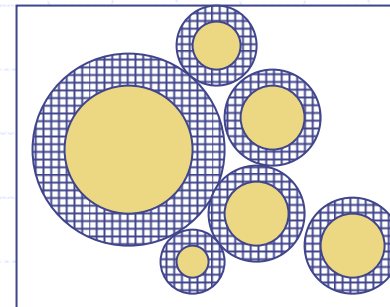


Optimal Microgeometries

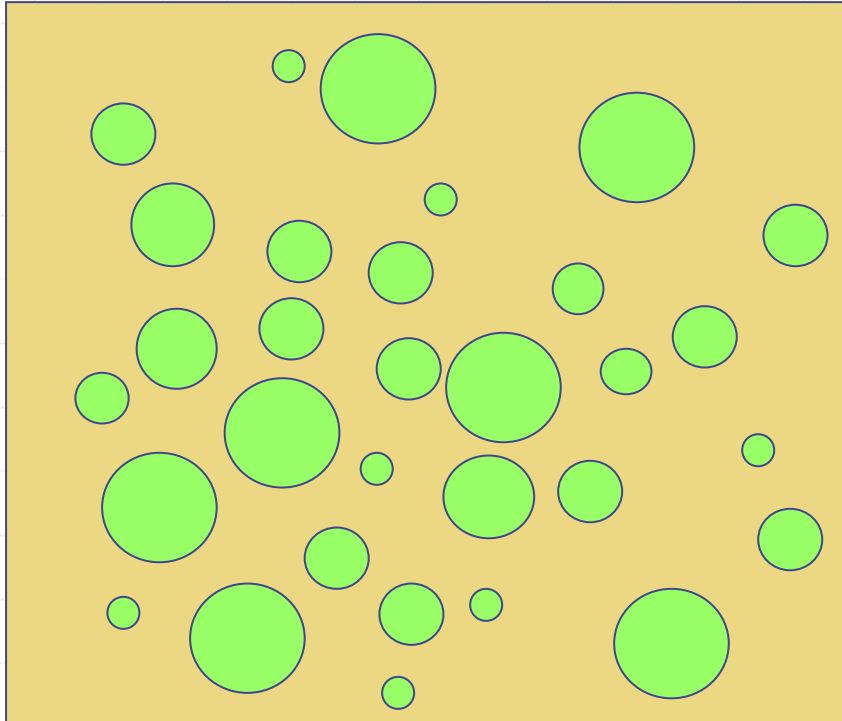
The lower bound is attained by the Hashin Shtrikman coated sphere assemblage with core of material one and coating of material two.



The upper bound is attained by the Hashin Shtrikman coated sphere assemblage with core of material two and coating of material one.



Bounds for effective thermal conductivity with coupled mass and thermal transport on the two-phase interface



Green spheres represent pores

Matrix is ceramic

Physical Process:

A temperature gradient is placed across porous ceramic

Impurities diffuse through matrix and release heat when arrive on surface of pore.

When impurities the leave pore surface and reenter matrix they absorb heat; this effect can enhances or decrease the effective conductivity of the porous ceramic.

Steady state coupled heat and mass transport inside the RVE

Thermal conductivity of the matrix σ_m

Thermal conductivity of the pore σ_p : $\sigma_p < \sigma_m$

Temperature inside the composite $T=T(y)$

Impurity concentration inside the composite $C=C(y)$

Impurity concentration on the pore surface

$$C_s = C_{s0} + a_T(T - T_0) + a_C(C - C_0)$$

C_{s0} , T_0 , C_0 are the equilibrium values and $a_T = \left(\frac{\partial C_s}{\partial T} \right)_{C_0, T_0}$ $a_C = \left(\frac{\partial C_s}{\partial C} \right)_{C_0, T_0}$

The surface diffusivity a_s has dimensions of length x diffusivity

The coefficient a_T is negative since C_s decreases with temperature

$$\Delta T = 0 \quad \Delta C = 0 \quad \text{inside each phase}$$

$$\mathbf{n} \cdot (\sigma_m \nabla T)_{matrix} - \mathbf{n} \cdot (\sigma_p \nabla T)_{pore} = -q D \mathbf{n} \cdot \nabla C \quad \nabla_S \cdot (a_S \nabla_S C_S) = -D \mathbf{n} \cdot \nabla C$$

q is specific heat release

Prescribed average temperature gradient \mathbf{E}

Boundary conditions: $T - \mathbf{E} \cdot \mathbf{x}$ is Q periodic, C is Q periodic.

Effective thermal conductivity

E Prescribed average temperature gradient across RVE

j Prescribed average heat flux across RVE

$$\mathbf{j} = \Sigma^E \mathbf{E}$$

Microgeometry known only statistically

It is supposed that the microgeometry is such that the effective conductivity is an isotropic tensor $\Sigma^E = \sigma^E \mathbf{I}$.

The microgeometry is composed of spherical pores of different radii. It is supposed that the volume fraction and size distribution of pore phase is known.

Since the matrix is a better conductor than the pore we seek to determine conditions on the pore size distribution and material properties for which $\sigma^E > \sigma_m$ and $\sigma^E < \sigma_m$

The effective conductivity with pore phase conductivity being perfect conductor is σ^∞ . The effective conductivity with pore phase insulator is σ^0 .

Interplay between microgeometry and material properties

Average pore radii $\langle a \rangle$

Harmonic average of pore radii $\langle a^{-1} \rangle^{-1}$

$$\text{If } \langle a^{-1} \rangle^{-1} \geq \frac{-2qa_s a_T}{\sigma_m - \sigma_p} - 2a_s \frac{a_c}{D} \left(\frac{\sigma^\infty - 1}{\theta_p} - 1 \right)^{-1}$$

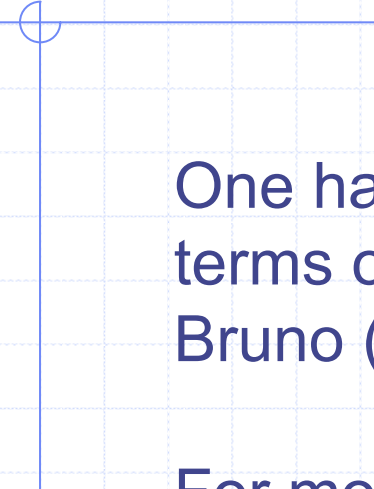
Then $\sigma^E \leq \sigma_m$ No enhanced conduction for sufficiently small surface to volume ratio

$$\text{If } \langle a \rangle \leq \frac{-2qa_s a_T}{\sigma_m - \sigma_p} - 2a_s \frac{a_c}{D} \left(\frac{1 - \sigma^0}{\theta_p} - 1 \right)$$

Enhanced conduction for surface to volume ratio sufficiently large

Then $\sigma^E \geq \sigma_m$

R. Lipton (1999)
JMPS (47)1699-1736



One has upper and lower bounds on σ^∞ and σ^0 in terms of lower bound on particle separation, Bruno (1991) P.Roy.Soc. Lond.(433)355-381.

For monodisperse suspensions see Torquato and Rubinstein J.App.Phys.(69)7118-712 for bounds on σ^∞ and σ^0 in terms of nearest neighbor distribution function.