# A MULTISCALE TECHNIQUE FOR THEORETICALCOMPUTATIONAL PREDICTION OF PROPERTIES OF HETEROGENEOUS MATERIALS 

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## TOPICS

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## INTRODUCTION (i)

- Generalities: Heterogeneous Media

Let us convince ourselves, simultaneously, that the heat transfer problem in heterogeneous media, in a general context, and the heat conduction problem in composite materials, in a specific context, are extremely old, relevant, challenging, interesting, and current problems!

We would like to understand, in fact, the macroscopic behavior of such media or materials, which depend on their 'effective properties.'

# Pioneering work by Lord Rayleigh, Phil. Mag., 1892. 

LVI. On the Influence of Obstacles arranged in Rectangular Order upon the Properties of a Medium. By Lord Rayleigh Sec. R.S.*

THE remarkable formula, arrived at almost simultaneously by L. Lorenz $\dagger$ and H. A. Lorentz $\ddagger$, and expressing th relation between refractive index and density, is well known but the demonstrations are rather difficult to follow, and th limits of application are far from obvious. Indeed, in som discussions the necessity for any limitation at all is ignored I have thought that it might be worth while to consider th problem in the more definite form which it assumes when th obstacles are supposed to be arranged in rectangular or squar order, and to show how the approximation may be pursues when the dimensions of the obstacles are no longer very small in comparison with the distances between them.

Taking, first, the case of two dimensions, let us investigate the conductivity for heat, or electricity, of an otherwise uniform medium interrupted by cylindrical obstacles which are art ranged in rectangular order. The sides of the rectangle wi l be denoted by $\alpha, \beta$, and the radius of the cylinders by $a$. Th d simplest cases would be obtained by supposing the material composing the cylinders to be either non-conducting or per* fectly conducting; but it will be sufficient to suppose that it has a definite conductivity different from that of the remainder of the medium.

Fig. 1.


Transport properties of regular arrays of cylinders

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(Communicated by R. H. Brown, F.R.S. - Received 20 February 1979 Revised 22 May 1979)


#### Abstract

We extend a method devised by Lord Rayleigh to enable the calculation of the transport properties of circular cylinders in square and hexagonal arrays. The theory is confirmed by measurements on arrays of perfectly conducting cylinders, and also is compared with asymptotic formulae due to Keller ( 1963 ) and $0^{\prime}$ Brian (1977). It is used to furnish plots of equipotential lines within the array. It is also applied to the calculation of the optical properties of films with columnar structure. Detailed studies for copper films show both the good solar selectivity possible with voided structures and the transition from a good reflector to a metal black consequent upon structural changes.


We give an analytic expression for the conductivity of this array in a similar form to Rayleigh (1892) based on square truncation to order $N=3$ :

$$
\begin{equation*}
\epsilon=1-2 f /\left[T+f-\frac{0.305827 f^{4} T}{T^{2}-\left(1.402958 f^{8}\right)}-\left\{\frac{0.013362 f^{8}}{T}\right\}\right], \tag{14}
\end{equation*}
$$

where $T$ is again defined by equation (13).
The term in curly brackets is the first correction term obtained from triangular truncation for order $N=4$. It is to be noted that Rayleigh failed to include the term in round brackets in his analytic expression based on the same order of summation. ${ }^{2}$

# Thermal Conductivities of a Cracked Solid 

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(Received January 18, 1983)


#### Abstract

Formulas are presented which describe the effect of flat elliptical cracks on the effective thermal conductivity of an oinerwise homogeneous body. The cracks are assumed randomly and isotropically distributed throughout the body, and may either be dry or composed of any material with a conductivity differing from that of the matrix. Effective conductivities depend solely upon a crack density parameter when the cracks are dry, and additionally upon a saturation parameter and the crack planform aspect ratio otherwise.


An analogy exists between $\sigma$, the electric conductivity, $J$ and $E$, the current and electric field vectors respectively, and between $k$, the thermal conductivity, and $q$ and grad 7 , the vector heat flow and temperature. Notice that in the governing equations describing the two phenomena, corresponding quantities in the following lists play identical roles:

| $\sigma$ | $k$ |
| :---: | :---: |
| $J$ | $q$ |
| $E$ | $\operatorname{grad} T$ |
| $J=\sigma E$ | $q=k(\operatorname{grad} T)$ |
| $\operatorname{div} J=0$ | $\operatorname{div} q=0$ |

In the same way, one can show that this analogous behavior persists in the specification of boundary conditions [3]. These observations imply that conclusions about electric behavior apply to thermal problems when the substitutions

$$
\begin{align*}
& J \rightarrow q \\
& E \rightarrow \operatorname{grad} T  \tag{1}\\
& o \rightarrow k
\end{align*}
$$

are carried out. Hoenig [3] has presented a study of the effects of cracks on the electrical conductivities of bodies. These results can be applied to thermal problems by means of the above substitutions. This analysis assumes that heat transfer across dry cracks by radiation or convection will not take place.

The problem of determining $k$ in (2) has been reduced by the above comments to the problem of evaluating the expression $(\operatorname{grad} T) / q \infty$ for a single crack and then averaging this expression over all orientations of the crack. The process of evaluation must somehow take into account the influence of the other cracks of the body; this is done by invoking a self-consistent hypothesis, initially articulated by Budiansky [6] and Hill [7]. According to their hypothesis, each crack in the matrix 'sees' itself as being embedded in an uncracked body, characterized however by the as-yet-unknown effective conductivity (that is, the macroscopic conductivity) of the cracked body. In this manner, the difficult problem of evaluating the right-most factor of (2) in the context of a crack subject to the complex influence of neighboring cracks is replaced by the substantially simpler one of evaluating this factor by considering a single crack in a specially defined but homogeneous matrix. An implicit assumption in this procedure is that the crack concentration is sufficiently small so that the effect of crack intersections can be neglected.

## HEAT AND MASS TRANSFER

IN REFRIGERATION AND CRYOGENICS

## - HEMISPHERE PUBLISHING CORPORATION

## Effective Thermal Conductivity of Frost

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Classical model for the effective conductivity of frost, 1987.

If a temperature gradient exists in a frost layer energy is transferred from the warm to the cold side by molecular conduction, by water vapcr diffusion, by radiation and occasionally by natural convection of the pore gas. A theoretical and experimental study has been carried out on the influence of these different transport mechanisms on the total energy flux in frost. This total energy flux can be represented by an effective thermal conductivity.


FIGURE 1. Heat and mass fluxes in a frost layer
is useful to separate the different effects by defining individual thermal conductivities

$$
\begin{equation*}
\lambda=-\frac{\dot{q}}{\mathrm{dT} / \mathrm{dx}} \tag{1}
\end{equation*}
$$

and to finally add all relevant individual conduvtivities to obtain an effective thermal conductivity of frost.

These few examples show that based on the criteria mentioned above only under extreme system conditions an influence of natural convection may occur. Normally, in real situations, it can be neglected. However, one has to take into account., that criteria (15) and (18) are valid for closed porous spaces, which in general is not the case with frost layers. Thus, a different behavior of the convective flux is possible. This should be studied by special experiments in the future.

## CONDUCTION

Molecular conduction in the ice matrix and in the pore space is by far the most important effect on the total heat flux. The thermal conductivicy of frost is not only a function of density and temperature but also of its internal structure.


FIGURE 9. Erost structure model
EFFECTIVE THERMAL CONDUCTIVITY
From, the foregoing considerations it follows that conduction and diffusion are the relevant effects on heat transfer in frost. The effective thermal conductivity is thus given by
$\lambda_{e f f}=\lambda_{C d}+\lambda_{D}$
with the thermal conductivity $\lambda_{D}$ due to diffusion according to eq. (10) (see Fig. 2) and the conduction thermal conductivity $\lambda$ cd from eq. (21) considering eqs. (14), (19), (20), (23), (24) and (25).

# Heat conduction characteristics of a carbon-fibre-reinforced lithia-alumino-silicate glass-ceramic 

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A study was conducted of the thermal diffusivity, specific heat and thermal conductivity of a uniaxially carbon-fibre-reinforced lithia-alumino-silicate glass-ceramic. The thermal diffusivity and conductivity parallel to the fibre direction was found to be independent of thermal history and more than an order of magnitude higher than in the transverse directions. During the first thermal cycle, the thermal diffusivity transverse to the fibre direction was found to exhibit a decrease attributed to crack formation under the influence of internal stresses. The transverse thermal diffusivity on thermal cycling to $1000^{\circ} \mathrm{C}$ exhibited lower values during heating than during subsequent cooling. This hysteresis was attributed to a thermal history-dependent barrier to heat flow at the matrix-fibre interface. The thermal conductivity of the fibres along their length inferred from composite theory was found to be much lower than the corresponding value for pyrolytic graphite, attributed to less than complete graphitization and associated high density of lattice defects which act as phonon scatterers.


Figure / Orientation of carbon-fibre reinforced lithium-aluminasilicate glass-ceramic.


Figure 2 Photomicrographs of carbon fibre-reinforced
lithia-alumino-silicate glass-ceramic at two different magnifications.

Schematic and micrograph of uniaxial carbon-fiber composite, 1987.

## THEORETICAL ANALYSIS

# Thermal Diffusivities of Composites with Various Types of Filler 

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#### Abstract

In-plane and out-of-plane thermal diffusivities (conductivities) of Kerimid resin composites reinforced with various types of filler were studied both experimentally and theoretically. The types of filler used are $\mathrm{SiO}_{2}$ particle, $\mathrm{Al}_{2} \mathrm{O}_{3}$ short fiber, Boron Nitride ( BN ) flake, and $\mathrm{Si}_{3} \mathrm{~N}_{4}$ whisker. The prediction based on our previous model (Eshelby's equivalent inclusion method) agreed reasonably well with the experiment, except for BN flake composite. It was found that the orientation of filler has a strong effect on the overall thermal conductivity of a composite.


Among these thermal properties, thermal diffusivity (or conductivity) has been studied analytically by a number of researchers, for example, References [6-10]. These analytical models are, however, aimed at simple geometries of filler microstructure, such as unidirectionally oriented continuous fiber and spherical particle composites. Thus, in this paper, the thermal diffusivity of composites with more complicated types of filler geometry is studied both experimentally and analytically.

Measured values of thermal diffusivity are compared with predicted values based on our model for thermal conductivity, $k_{c}$, of a misoriented short fiber composite $[3,4]$.

The orientation distribution of the filler can be easily estimated by considering that all the composite samples were formed by compression molding. That is to say, short fiber and whisker composites can be considered to be nearly twodimensional ( 2 D random) and flake composites, unidirectional. The thermal conductivity of a composite reinforced with fillers of given orientation type can be predicted by our model based on Eshelby's equivalent inclusion model [3,4]. In this model, actual fillers with thermal conductivity $k_{f}$ in a composite are replaced by equivalent inclusions which possess the same thermal conductivity as the surrounding matrix, $k_{m}$, and eigen-temperature gradient. Thus, the model is similar to that developed originally for elasticity problems [17,18]. The present study includes:

1. Spherical particle reinforced composite ( $\mathrm{SiO}_{2}$ particle/Kerimid)
2. In-plane random short fiber reinforced composite ( BN flake/Kerimid)
3. 2D random short fiber reinforced composite $\left(\mathrm{Al}_{2} \mathrm{O}_{3}\right.$ short fiber/Kerimid,

- $\mathrm{Si}_{3} \mathrm{~N}_{4}$ whisker/Kerimid)

4. Nearly three-dimensional (3D random) short fiber reinforced composite $4\left(\mathrm{Si}_{3} \mathrm{~N}_{4}\right.$ whisker/Kerimid)

## EXPERIMENTAL APPARATUS AND PROCEDURE

## Sample Selection and Preparation

Four kinds of fillers and heat resistant polymers (Table 1) which exhibit relatively high thermal conductivity, were chosen for the reinforcement and matrix, respectively.|

In the selection process, special attention was placed upon covering a wide range of filler geometry, i.e., from flake to short fiber. The raw materials were processed into composite materials by two kinds of compression molding methods, the premix method and the paper making method,

It should be noted in the figure that, except for BN/Kerimide composite [Figure 8(c)], the predicted values of $\lambda_{z}$ and $\lambda_{x y}$ agree reasonably well with the experimental values when the volume fraction of the filler $V_{f}$ is small, but overestimate the experimental values as $V$, becomes large.

# Theoretical model accounting for radiation and conduction, 2000. 

## Conduction and Radiation Heat Transfer in High-Porosity Fiber Thermal Insulation

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Radiation is the primary mode of heat transfer in high-porosity fiber thermal insulations even at temperatures above a few hundred Kelvin. Consequently, many studies have reported on the modeling of radiation heat transfer through high-porosity fibrous media.

Heat transfer by combined radiation and conduction in fibrous media has been addressed by many investigators using a simple additive model in terms of the thermal conductivities for radiation and conduction; the latter includes conduction through the solid lattice of the fiber medium and any gas present in the insulation.f

The present theoretical raliationmodel includes formulations for radiative properties and thermal conductivity of fibrous media.

## Conduction Heat Transfer

Although the dominant mode of heat transfer through highporosity fiber thermal insulations is generally radiation, the contributions of conduction through the solid phase, i.e., fibers, and any gas present in the void space between the fibers must be accounted for when comparing theoretical predictions with measured heat-transferdata.|

In the limit of large optical thickness, Eq. (35) reduces to

$$
\begin{equation*}
k_{e}=k_{r}+k_{t} \tag{39}
\end{equation*}
$$

indicating that heat transfer by radiation and conductionare additive for optically thick media.


Fig. 3 SEM of bonded fibers; magnification $=1200 \mathrm{X}$.

## Experimental measurements of radiative (and conductive) properties, 2000.

## Determination of Spectral Radiative Properties of Open Cell Foam: Model Validation

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Spectral radiative propertis (absorption coefficient, scattering coefficient, and phase function) of open cell carbon foam are determined experimentally. The identification method uses spectral transmittance and reflectance measurements and a prediction model based on a combination of geometric optics laws and of diffraction theory. In the wavelength region of $0.1-2.1 \mu \mathrm{~m}$, directional-hemispherical transmittance and reflectance measurements are used, whereas directional-directional transmittance and reflectance measurements are used in the wavelength region of $2-15 \mu \mathrm{~m}$. Thus, radiative properties are determined in the wavelength region from visible to infrared. The two approaches corresponding to the two different types of measurement (directional-directional and directionalhemispherical) are compared for the determination of radiative properties. Moreover, experiments performed on a guarded hot-plate-type device are used to confirm that the proposed model is appropriate to predict the radiative heat transfer in such media

Open cell carbon foam can be used as efficient thermal insulation for high-temperature applications. Insulating foam consists of a highly porous solid material. Open cell foam insulations are semitransparent media (absorbing, emitting, and scattering radiation).

To model heat transfer in such media, it is necessary to determine radiative and conductive properties.

The total conductivity includes the three independent mechanisms: conduction through the gas, conduction through the solid material forming the cell, and thermal radiation ${ }^{13-15}$ :

$$
\begin{equation*}
k_{1}=k_{\text {gas }}+k_{\text {solid }}+k_{r} \tag{7}
\end{equation*}
$$

## Effective Thermal Conductivity of Saturated'

## Sintered Nicke! Loop Heat Pipe Wicks

## by

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## Abstract

In this investigation, the effective thermal conductivity of sintered metal wicks was studied both experimentally and analytically. The experimental study consisted of measuring the effective conductivity of eleven samples in vacuum and with three different saturating fluids (air, water and methanol). The analytical study aimed to find a model to better predict the effective conductivity. The wicks tested were typical of loop heat pipas for spacecraft thermal control systems. The data obtained using the different fluids allows the effective thermal conductivity to be predicted as a function of other saturating fluids. The measured values for effective thermal conductivity were compared with other typically measured parameters for loop heat pipe wicks, including the porosity, permeability, pore radius, and compression load.


Figure 1: Basic Loop Heat Pipe [2]
Models of Effective Thermal Conductivity

a)

Direction of Heat Transfer

b)

Figure 2 a) liquid and solid in series, b) liquid and solid in paralle! [4]
a)


b)

Effective Thermal Conductivity of Liquid Saturated Sintered Fiber Metal Wicks

The error on the measurement of the thermal resistarice of the wick was less than $9.1 \%$ as shown by calculations.

## Overall Results

Comparison was made between the mentioned basic models for the effective conductivity and the experimental results. Most models were unable to accurately predict the effective conductivity, both in dry and saturated states.

One item to note is that the correlations typically only use the sample porosity to vary the effective conductivity. This results in significant lost information regarding the sample structure.

## Experimental measurements of effective conductivity of heat pipe wicks, 2004.

Conclusions and Recommendations


c)

In future work, additional measurements of the effective conductivity with variations in the metai material and an alternate to water would be jeneficial. As for development of a correlation, information regarding the structure of the samples is seen as vital. This information consists of the particle size distribution and general particle geometry (it is assumed the particles are not really spherical based on the current results of the measurements).

Figure 3 : a) unit cell, b) a quarter of the unit cell, c) heat resistance schematic [7]

# Microstructural Modeling and Thermal Property Simulation of Unidirectional Composite 

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The electrical, thermal and mechanical properties of functionally graded materials vary with microstructure and composition. Consequently it is very important to know quantitatively the properties of composites for the design of functionally graded materials. However few methods of quantitative and theoretical evaluation for material properties on wide compositional range have been established. In this research, a method that estimates the material properties of composites directly from their microstructure assisted with finite element analysis was investigated. As an example of the estimation of material properties, the thermal conductivity of Mo fiber-Cu matrix composites has been evaluated. Calculated results of thermal conductivity are well in agreement with the experimental data measured by using a laser flash apparatus and the smallest deviation is $1.9 \%$. The finite element analysis using a metallographic model is a very accurate method for estimation of composite properties.
geometric modeling technique $\frac{\text { Digital Image Based (DIB) }}{(0,12)}$ was used io reflect the actual morphology of composite microstructure such as inclusion shape, volume fractions, etc. on Finite Element (FE) model. The DIB technique for 2-dimensional models can be divided into three parts.
This DIB technique has a great advantage of excluding any meshing manipulation such as defining coordinates and element connectivities'because all the elements have the same size.

Fabrication and evaluation of Mo fiber-Cu matrix composite
Mo fiber-Cu matrix composite specimens were prepared from Mo fibers with a diameter of $120 \mu \mathrm{~m}$ and Cu plates.


(a)


Tho model of unidirectional circular cylinders packed in square arrays is shown as an ideal unidirectional composite in Fig. 3. From this ideal model, it is assumed that (a) the composites are macroscopically homogeneous, (b) locally, both the matrix and the fiber are homogeneous and isotropic, (c) the thermal contact resistance between the fiber and matrix is negligible, (d) the problem is two-dimensional, and (e) the fibers are arranged in a square periodic array, i.e. they are uniformly distributed in the matrix. The model shown in Fig. 3(a) is a unit cell which represents one-cycle of the periodic structure, so the transverse thermal conductivity of unidirectional composite of circular cylinders was estimated by using this unit cell. The unit cell was divided into 4 -node fixed size square elements as shown in Fig. 3(b), so that the FE model obtained from the unit cell became equivalent to that obtained from the microstructure of composites.

## Comparison

The fibrous and transverse thermal conductivities of the specimens were plotted respectively in Fig. 11, where the volume fraction of molybdenum was determined to be $88 \%$ from the density measured by Archimedes's method. The experimental thermal conductivity along the fiber direction was compared with the pararell model in Fig. 11(a), while for the transverse direction it was compared with the Perrins's model in Fig. 11 (b). The pararell model is a linear rule of mixtures, while the Perrins's model is a predictive model for the transverse circular cylinders packed in hexagonal arrays. Each experimental result is well in agreement with the predicted one, so there is no thermal barrier at the interfaces, which is also obvious from the SEM micrographs.

Fig. 3 The schematic illustration of the unidirectional model for circular cylinders packed in square arrays. (a) a unit cell. (b) the schematic :.illustration of FE model based on unit cell (a).

COMPOSITE STRUCTURES

Multiscale modelling of thermal conductivity in composite materials for cryogenic structures

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Multiscale modeling of thermoelastic behavior
of braided fabric composites for cryogenic
structures
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Abstract

A multiscale analysis is performed to estimate the thermomechanical behavior of a column-type support post used in particle acoelerators to sustain cryomagnets.

## INTRODUCTION (ii)

- Objectives

Development and application of a multiscale theoreticalcomputational approach to calculate the effective conductivity of composite materials with 2-D or 3-D microstructures, and with or without the presence of voids, and of an interfacial thermal resistance between the constituent phases.

- Motivation

Engineering applications of composite materials in various industries (electronic equipment, aerospatial, nuclear etc.).
$>$ Relatively easy to fabricate.
$>$ Low cost and low weight.
$>$ Desirable/tailorable mechanical, thermal, and electrical properties (stiffness, resistance to corrosion and wear, thermal expansion coefficient, electrical and thermal conductivity, dielectric constant).

## INTRODUCTION (iii)

- Problem of interest

Steady state heat conduction in composite materials.

- Definition of composite materials
$>$ Fabricated heterogeneous media with two or more phases that possess distinct macroscopic properties.
$>$ Continuous phase: matrix (constituted by metallic, organic, or ceramic materials).
$>$ Dispersed phase: particles and/or fibers (silicon carbide, aluminum oxide, carbon, graphite), voids.
- 'Classification’ of composite materials
$>$ Particulate (particles, [approx.] spherical, ellipsoidal etc.).
$>$ Fibrous (e.g., fibers with axisymmetric geometry).
$>$ Hybrid (mixture of particles and fibers).


## Carbon Fiber Composites

Deborah D. L. Chung<br>Butterworth-Heinemann © 1994

Boston London Oxford Singapore Sydney Toronto Wellington

Composite materials refer to materials containing more than one phase such that the different phases are artificially blended together.

A composite material typically consists of one or more fillers in a certain matrix. A carbon fiber composite refers to a composite in which at least one of the fillers is carbon fibers, either short or continuous, unidirectional or multidirectional, woven or nonwoven. The matrix is usually a polymer, a metal, a carbon, a ceramic, or a combination of different materials. 1

Polymer-matrix composites are much easier to fabricate than metalmatrix, carbon-matrix, and ceramic-matrix composites, whether the polymer is a thermoset or a thermoplast.'

Carbon fiber metal-matrix composites are gaining importance because the carbon fibers serve to reduce the coefficient of thermal expansion (Figure 7.1 [1]), increase the strength and modulus, and decrease the density. If a relatively graphitic kind of carbon fiber is used, the thermal conductivity can be enhanced also (Figure 7.2 [2]).

Carbon fibers used for metal-matrix composites are mostly in the form of continuous fibers, but short fibers are also used.|

Carbon is the matrix that is most compatible to carbon fibers.
In addition to having attractive mechanical properties, carbon-carbon composites are more thermally conductive than carbon fiber polymer-matrix composites.

Carbon-carbon composites with high thermal conductivity are important for first wall components for nuclear fusion reactors, hypersonic aircraft, missiles and spacecraft, thermal radiator panels, and electronic heat sinks.

## Book on carbon fiber composites: thermal applications and issues, 1994.

Carbon fibers are electrically and thermally conductive, in contrast to the nonconducting nature of polymer and ceramic matrices. Therefore, carbon fibers can serve not only as a reinforcement, but also as an additive for enhancing the electrical or thermal conductivity. Furthermore, carbon fibers have nearly zero coefficient of thermal expansion, so they can also serve as an additive for lowering the thermal expansion. The combination of high thermal conductivity and low thermal expansion makes carbon fiber composites useful for heat sinks in electronics and for space structures that require dimensional stability. As the thermal conductivity of carbon fibers increases with the degree of graphitization, applications requiring a high thermal conductivity should use the graphitic fibers, such as the high-modulus pitch-based fibers and the vapor grown carbon fibers. Carbon fibers are more cathodic than practically any metal, so in a metal matrix, a galvanic couple is formed with the metal as the anode. This causes corrosion of the metal. The corrosion product tends to be unstable in moisture and causes pitting, which aggravates corrosion. To alleviate this problem, carbon fiber metal-matrix composites are often coated.

## Thermal Conductivity

The thermal
conductivities of P-100, P-120, and K1100X fibers are all higher than that of copper, while the thermal expansion coefficients and densities are much lower than those of copper. Thus, the specific thermal conductivity is exceptionally high for these carbon fibers.

In contrast, vapor grown carbon fibers have a thermal conductivity of $1900 \mathrm{~W} / \mathrm{m} / \mathrm{K}$ at $25^{\circ} \mathrm{C}[76]$. Hence, carbon-carbon composites using vapor grown carbon fibers may have a thermal conductivity exceeding $1000 \mathrm{~W} / \mathrm{m} / \mathrm{K}$ [77]. The low density of carbon makes the specific thermal conductivity of carbon-carbon composites outstandingly high compared to other materials. The use of porous carbon-carbon composites with even lower densities [78] may further increase the specific thermal conductivity.

## InTERFACE

Therefore, an optimum degree of fiber-matrix bonding is needed for brittle-matrix composites, whereas a high degree of fiber-matrix bonding is preferred for ductile-matrix composites.

The mechanisms of fiber-matrix bonding include chemical bonding, van der Waals bonding, and mechanical interlocking.

## INTRODUCTION (iv)

- Effective thermal conductivity (second order tensor)
"Ratio" between volumetric mean of heat flux to volumetric mean of temperature gradient for a representative volume element (Milton, 2002):

$$
\begin{gathered}
\langle\mathbf{q}\rangle=\mathbf{K}_{\text {eff }}\langle\nabla T\rangle \\
\langle\mathbf{q}\rangle \equiv \frac{1}{V} \int_{V} \mathbf{q}(\mathbf{x}) d V=\frac{1}{V}\left(\int_{V_{m}} \mathbf{q}_{m}(\mathbf{x}) d V+\int_{V_{d}} \mathbf{q}_{d}(\mathbf{x}) d V\right) \\
\langle\nabla T\rangle \equiv \frac{1}{V} \int_{V} \nabla T(\mathbf{x}) d V=\frac{1}{V}\left(\int_{V_{m}} \nabla T_{m}(\mathbf{x}) d V+\int_{V_{d}} \nabla T_{d}(\mathbf{x}) d V\right) \\
(m-\text { matrix; } d-\text { dispersed phase })
\end{gathered}
$$

## INTRODUCTION (v)

- Microstructure

Geometrical arrangement of the composite phases; characterized by the volume fraction and by the spatial, size, orientation, and shape distributions of the dispersed phase(s) inside the matrix; the microstructure may or may not be statistically homogeneous $(\Rightarrow$ dispersed phase volume fraction independent of position).

- Classification for modeling purposes
$>$ With respect to spatial distribution of the phases:
$\checkmark$ Ordered (distribution function is 'trivial');
$\checkmark$ Random (distribution function is 'non-trivial').
$>$ With respect to periodicity:
$\checkmark$ Periodic (representative volume element, or cell, repeats itself along the spatial directions);
$\checkmark$ Non-periodic.


## INTRODUCTION (vi)

- Illustration of 2-D microstructures
(dispersed phase: cylinders of 'infinite' length)

one-particle cell

multi-particle cells




Figure 9 Crack formation in uniaxial carbon fibre reinforced lithia-dumino-silicate glass-ceramic annealed for 4 h at $1000^{\circ} \mathrm{C}$.

## INTRODUCTION (vii)

- Illustration of 3-D microstructures
(dispersed phase: spheres)



## Review

 The physical properties of composite materials算

D. K. HALE

microstructural
geometries


b

$d$

Figure 1 Composite geometries: (a) random dispersion of spheres in a continuous matrix, (b) regular array of aligned filaments, (c) continuous laminae, (d) irregular geometry.

## micrograph of tooth



Figure 9 Scanning electron micrograph (X 100) showing marginal gap produced by difference in thermal expansion coefficients of dental filling material and tooth substance (courtesy Dr W. Finger).

# Determination of the thermal conductivity and diffusivity of thin fibres by the composite method <br> Determination of properties 

2.3. Evaluation of the thermal conductivity and diffusivity of the fibres from composite theory
For heat-flow parallel to uniaxially aligned fibres, the thermal conductivity, $K_{\mathrm{c}}$, of a composite is
where $K$ is the thermal conductivity, $V$ is the volume-fraction and the subscripts $c, m$ and $p$, refer to the composite, matrix and fibres, respectively.
For heat-flow perpendicular to the fibre direction, the thermal conductivity, as derived by Bruggeman [7], can be written

$$
\begin{equation*}
\left(\frac{K_{\mathrm{m}}-K_{\mathrm{c}}}{K_{\mathrm{m}}+K_{\mathrm{c}}}\right) V_{\mathrm{m}}=\left(\frac{K_{\mathrm{c}}-K_{\mathrm{p}}}{K_{\mathrm{c}}+K_{\mathrm{p}}}\right) V_{\mathrm{p}} . \tag{2}
\end{equation*}
$$

From the measured value of the thermal diffusivity, the corresponding value of the thermal conductivity, $K$, can be calculated from

$$
\begin{equation*}
K=\kappa \rho c, \tag{3}
\end{equation*}
$$

where $\kappa$ is the thermal diffusivity, $\rho$ is density and $c$ is the specific heat. The specific heat of the composite can be calculated from the measured values for the specific heat of the fibres and the matrix by means of the rule of mixtures. Substitution of the values for the thermal conductivity of the matrix and the composite into Equation 1 or 2 permits calculations of the thermal conductivity of the fibres. The thermal diffusivity may then be determined using Equation 3.

[^0]
## INTRODUCTION (viii)

- Interfacial thermal resistance
$>$ Origin: fabrication process.
$>$ Causes: poor mechanical and/or chemical adherence; presence of impurities and roughness; difference between the thermal expansion coefficients of the phases; cracks.
$>$ Effect: jump of the temperature field at the interface between the phases (barrier to heat conduction).
$>$ Definition/model: ratio between the temperature jump to the heat flux at the interface:

$$
R_{I} \equiv \frac{\left.T_{m}\right|_{\text {interface }}-\left.T_{d}\right|_{\text {interface }}}{\left.q\right|_{\text {interface }}}\left[\mathrm{m}^{2} \cdot \mathrm{~K} / \mathrm{W}\right] ; \quad h_{s} \equiv \frac{1}{R_{I}}\left[\mathrm{~W} / \mathrm{m}^{2} \cdot \mathrm{~K}\right]
$$

## Role of Interfacial Debonding and Matrix Cracking in the Effective Thermal Diffusivity of Alumina-Fiber-Reinforced Chemiçal-Vapor-Infiltrated Silicon Carbide Matrix Composites

Department of Materials Engineering, Virginia Polytechnic Institute and State University,
Evidence of interfacial debonding

## and matrix cracking, 1991. <br> * H. Tawil <br> Societe Europeenne de Propulsion, Les Cinq Chemins-Le Haillan, F 33165 Saint Medard en Jalles

The thermal diffusivity of a biaxial weave alumina-fiberreinforced chemical-vapor-deposited (CVD) SiC composite heated to $1500^{\circ} \mathrm{C}$, which is above the manufacturing temperature, was found to exhibit an increase for heat flow parallel to the fiber plane, whereas a decrease was observed perpendicular to the fiber plane. The increase parallel to the fiber plane was thought to be due to the annealing of the fibers and matrix. The decrease perpendicular to the fiber plane was found to be the result of interfacial debonding and matrix cracking within the plane of the fibers. [Key words: composites, fiber reinforcement, chemical vapor deposition, thermal diffusivity, cracking.]

## I. Introduction

Ceramic matrix composites offer considerable advantage over monolithic single-phase ceramics for high temperature applications, in view of their enhanced fracture toughness, noncatastrophic failure mode, and increased thermal shock resistance. From the perspective of thermal insulation, temperature control, and energy conservation, information on the variables which control the effective thermal conductivity of ceramic matrix composites is critical for purposes of design, materials selection, and performance prediction of high-temperature structures and components.
II. Experimental Procedure and Results

Figure 1 shows a SEM micrograph of a polished cross section perpendicular to the fiber direction prior to thermal property measurement. The fiber volume fraction was approximately $42 \%$. The presence of a few pores within the SiC matrix indicates that the infiltration process was nearly fully complete.

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It is suggested that the matrix cracking and interfacial debonding shown in Fig. 9 are related to the differences in the coefficient of thermal expansion which for the alumina exceeds the corresponding value for the silicon carbide.

The resulting preferred crack orientation will primarily affect the thermal diffusivity transverse to the fiber plane.


#### Abstract

This mechanism is offered as an explanation for the lower value for the thermal diffusivity in vacuum than in nitrogen or helium, as shown in Fig. 8. Furthermore, it also presents proof that interfacial and matrix cracks can act as insuiators, especially under vacuum. Indirect support for the above explanations is provided by the data of Eckel and Bradt, ${ }^{19}$ who observed a hysteresis in the thermal expansion behavior of composites similar to those of the present study, which was also attributed to interfacial debonding due to the thermal expansion mismatch.


Comparison of the data of Figs. 7 and 8 suggests that heating to $1500^{\circ} \mathrm{C}$ has introduced a structural change of a type such that the ambient gaseous atmosphere affects only heat flow transverse to the fiber direction.

This micrograph clearly indicates the existence of crack formation coupled with interfacial separation within the plane of the fibers. Because cracks do not affect heat conduction parallel to the fiber plane, ${ }^{18}$ only the effective thermal conductivity transverse to the plane of the cracks, i.e., transverse to the fiber plane, is expected to be affected, in agreement with the data shown in Figs. 7 and 8. SEM fractographs of samples heated to $1500^{\circ} \mathrm{C}$ were similar to the one shown in Fig. 2, again showing that crack propagation occurred preferentially along the fiber-matrix interface.


The interfacial spacing and the matrix crack opening displacement is such that the gaseous heat transfer is in the socalled "molecular regime," in which the mean free path between collisions of the gaseous species with one another is much larger than the gap or crack width. ${ }^{20}$

As a final general remark, the results of this reinforce the findings of earlier studies ${ }^{15,17}$ that the measurement of the heat conduction behavior of solids in different gaseous environments can be used as a test for microstructural damage by nondestructive means.

Fig. 9. SEM micrograph of polished section of alumina-fiberreinforced CVD SiC matrix composite heated to $1500^{\circ} \mathrm{C}$ in nitrogen, showing evidence of interfacial debonding and matrix cracking.

# Effective Thermal Conductivity and Thermal Contact Conductance of Graphite Fiber Composites 

S. R. Mirmira, ${ }^{*}$ M. C. Jackson, ${ }^{\dagger}$ and L. S. Fletcher ${ }^{\ddagger}$ Texas A\&M University, College Station, Texas 77843-3123


#### Abstract

The transverse and longitudinal effective thermal conductivity and contact conductance of discontinuous and misoriented graphite fiber-reinforced composites has been studied over a range of temperatures ( $20-200^{\circ} \mathrm{C}$ ) and pressures ( $172-1720 \mathrm{kPa}$ ). Three different fiber types (DKE X, DKA X, and K22XX) and three fiber volume fractions ( 55,65 , and $75 \%$ ) in a cyanate ester matrix were studied. The addition of fibers to the matrix resulted in an increase in effective thermal conductivity, but appears to level off at fiber volume fractions of $65 \%$. Furthermore, the effective thermal conductivity in the longitudinal direction was significantly greater than in the transverse direction and was more dependent on temperature. These data were used to develop an equation relating the thermal contact conductance to the harmonic mean thermal conductivity of the fiber and matrix material, fiber volume fraction, sample thickness, and microhardness.




Figure 4.10. Magnified cross section of K22 XX fiber exhibiting a definite texture.

Measurements of effective conductivity, acknowledging presence of interfacial resistance and voids, 1999, 2001.
EFFECTIVE THERMAL CONDUCTIVITY OF FIBROUS COMPOSITES:

EXPERIMENTAL AND ANALYTICAL STUDY
A Dissertation
by

SRINIVAS RANGARAO MIRMIRA
Submitted to the Office of Graduate Studies of Texas A\&M University in partial fulfillment of the requirements for the degrec of DOCTOR OF PHILOSOPHY

December 1999


Table 1 Theoretical models for effective thermal conductivity of graphite composites


Chamis ${ }^{14}$

$$
k_{e}=\left(1-\sqrt{V_{f}}\right) k_{m}+\frac{k_{m} \sqrt{V_{f}}}{1-\sqrt{V_{f}}\left(1-k_{m} / k_{f}\right)}
$$

Hatta and Taya ${ }^{1 \text { : }}$

Caruso and Chamis ${ }^{16}$

Mottram and Taylor ${ }^{17}$

$$
\frac{k_{e}}{k_{m}}=\left(\left\{\sqrt{\left[\left(1-\frac{v_{f}}{1-V_{p}}\right)^{2}\left(\frac{k_{f}}{k_{m}}-1\right)^{2}+\frac{4 k_{f}}{k_{m}}\right]}\right.\right.
$$

$$
\left.\left.-\left(1-\frac{V_{f}}{1-V_{p}}\right)\left(\frac{k_{f}}{k_{m}}-1\right)\right\}^{2} / 4\right)\left(1-V_{p}\right)\left(\frac{x+1}{x}\right)
$$

Hasselman and Johnson ${ }^{18}$

$$
k_{e}=k_{m}\left[1+v_{f} /\left(\frac{1-v_{f}}{3}+\frac{k_{m}}{k_{f}-k_{m}}\right)\right]
$$

$$
k_{e}=\left(1-\sqrt{V_{f}}\right) k_{m}+\frac{k_{m} \sqrt{V_{f}}}{1-\sqrt{V_{f}}\left(1-V_{m} / V_{f}\right)}
$$

$x=2$ for spheres
$=1$ for cylinders perpendicular to heat flow
$k_{e}=k_{m}\left\{\left[2 v_{f}\left(\frac{k_{f}}{k_{m}}-\frac{k_{f}}{r h_{i}}-1\right)+\frac{k_{f}}{k_{m}}+2 \frac{k_{f}}{r h_{i}}+2\right] /\right.$

$$
\left.\left[v_{f}\left(1-\frac{k_{f}}{k_{m}}+\frac{k_{f}}{r h_{i}}\right)+\frac{k_{f}}{k_{m}}+2 \frac{k_{f}}{r h_{i}}+2\right]\right\}
$$

Based on this review, it appears that modeling the effective thermal conductivity of fiber composites should account for the geometrical arrangementof the fibers, the dimensions of the fibers, the fiber volume fraction, and thermal conductivity of the fiber and matrix. The model should also account for the interfacial thermal resistance between the fiber and the matrix and the possibility of transversely anisotropic fibers.

## Experimental Program

To provide additional experimental data on the effective thermal conductivity and thermal contact conductance of discontinuous graphite fiber composites, under controlled conditions, an experimental program was undertaken. The following sections describe the materials selected, the test facility, experimental procedure, and the uncertainty associated with results.
To avoid convection losses, the entire test facility was housed in a vacuum of $1 \times 10^{-5}$ torr maintained by an oil diffusion pump backed by a two-stage rotary pump. Further, radiative losses from the fluxmeters and samples were reduced by placing a segmented radiation shield around the vertical test column.

## Conclusions

On one
hand, the transverse effective thermal conductivity of the composites was highest for fiber volume fractions of $65 \%$, above which the increased interfacial thermal resistance between the fiber and matrix negated any benefit due to greater fiber volume. On the cther hand, the longitudinal effective thermal conductivity increased for higher fiber volume fractions. The longitudinal thermal conductivity was approximately one order of magnitude greater than the transverse. Furthermore, the effective thermal conductivity of the composites did not vary significantly over the selected temperature range.]

Considering the importance of the interfacial thermal resistance between the fiber and the matrix, it is recommended that a fundamental experiment be conducted (ideally with known number of fibers) to quantify this value as a function of material properties. It is also recommended that the effect of cryogenic temperatures on the thermal conductivity be examined and a largerrange of fiber volume fractions be tested. Further, it is apparent that the present models do not accurately predict the thermal conductivity of graphite composites. It would be beneficial to develop a model that accounts for the various influencing parameters, including the interfacial thermal resistance between the fibers and the matrix. Electron microscopy studies would reveal the nature of bonding between the fibers and the matrix, as well as the presence of voids.

## Critique of previous <br> approaches, 1999, 2001.

# Numerical simulation of thermal conductivity of MMCs: effect of thermal interface resistance 

D. Duschlbauer, H. J. Böhm and H. E. Pettermann

The thermal conductivity of metal matrix composites is investigated by computational simulations, in which the effect of a thermal barrier resistance between the constituent phases is explicitly taken into account. A numerical unit cell approach, which is based on the finite element method, an analytical mean field method of the Mori Tanaka type and bounding techniques are employed. To predict the effective conductivities oir fibre composites two different types of unit cell are utilised for the numerical studies. Two dimensional unit cells are developed which allow for investigations of aligned, continuous fibre reinforced composites while three dimensional unit cells are employed to study a large variety of different arrangements of non-staggered and staggered aligned short fibres. In the case of short fibres the th irmal barrier resistances of the end faces and of the cylindrical surfaces are modelled independently, which allows one to study both their individual and their combined influences on the overall behaviour. Results are presented for carbon fibre/copper composites and their overall thermal conductivities are investigated in terms of interfacial thermal barriers and microtopologies.

MST/5341

## Introduction

Metal matrix composites (MMCs) are widely used in electronic packaging applications, because of the possibility of tailoring the properties of the composite. The coefficient of thermal expansion (CTE) and thermal conductivity are the two most important design parameters.

Because of copper's non-reactivity with carbon, a drawback of carbon-copper composites is the poor matrix/fibre interface, which severely reduces the effective heat flow passing through the interface.

Due to different morphologies of carbon fibres' end faces and cylindrical surfaces (side faces) but also due to breaking of carbon fibres (e.g. during the hot pressing process of precoated fibres, leaving fibres with coated side faces and non-coated end faces, , high risk and low risk areas of potential thermal interface degradation are created. It is an aim of the present investigation to determine the effects of interface failure on the effective conductivity.

$$
\begin{aligned}
& \text { 2-D ANSYS simulation } \\
& \text { accounting for interfacial } \\
& \text { resistance, } 2003 \text {. }
\end{aligned}
$$

Numerous models have been published for predicting the effective transport properties of heterogeneous media. The majority of the analytical estimates have been based on the equivalent inclusion method dealing with inclusions of ellipsoidal shape. In this basic form these models assume ideal thermal contact between the constituents, ${ }^{3-6}$ and extensions for modelling coated inclusions have been reported. ${ }^{7.8}$ The implementation of non-ideal thermal interfaces where the temperature field is not continuous at constituent faces ${ }^{9,10}$ represents another group of extended models.

The interfacial thermal barrier was modelled as a layer of small (but finite) thickness and poor conductivity, i.e. introducing a third phase.

In the present work, numerical unit cell studies focus on aligned CFRCs and aligned, short fibre reinforced composites (SFRCs). In the case of CFRCs, regular fibre arrangements as well as random fibre arrangements are investigated. SFRCs are studied with respect to the influence of axial fibre offset and the degree of stagger on the effcctive conductivity. For both CFRCs and SFRCs the influence of thermal barriers at the fibre/matrix interfaces on the effective conductivity is investigated by means of appropriate thermal interface elements. For the analytical studies a Mori - Tanaka type approach for coated inclusions is used, which is applicable to the case of thermal interfacial resistances as well.|

## Thermal interface barrier

An interfacial thermal barrier between matrix and fibre may arise because of poor mechanical contact, the presence of impurities at the interface or debonded regions.

Unlike earlier work, ${ }^{11.12}$ where the thermal interfacial barrier was implemented into FEM via an interphase of low conductivity, in the present work the thermal interfacial barrier is implemented as an interface within the unit cell approach. Specific thermal contact surface elements are employed at the constituent interfaces.
composite with fixed volume fraction, skin constant, inclusion shape and orientation, containing large inclusions exhibits a higher, effective conductivity than would be the case for smaller inclusions due to the fact that the ratio of inclusion surface area (i.e. the interfacial area) to volume decreases as the inclusion size increases. ${ }^{10}$

## Unit cell approach

The unit cell approach describes the macroscale and microscale behaviour of inhomogeneous materials by studying model materials that have idealised periodic microstructures.


1 Two dimensional unit cells for periodic arrangement (rectangular) of aligned continuously reinforced composites: fibre volume fraction $\zeta=0.4$ |

## UNIT CELLS FOR CONTINUOUSLY FIBRE REINFORCED COMPOSITES

Clearly these regular
arrange $e_{i}$ ents do not fully represent 'real' composites. Improved models can be obtained with multifibre unit cells in which fibre positions are selected randomly or taken from micrographs. In the present study a unit cell with pseudorandom fibre positions is used, which is based on an arrangement used earlier ${ }^{21}$


If some microtopology shows a set of parallel symmetry planes, these planes have special properties.

Symmetry BCs are very useful for describing simple, regular microgeometries, but they are less suited to model random arrangements. On the one hand a random arrangement suitable for symmetry BCs is only pseudorandom as the fibres may either not touch a face or must be bisected by one or more faces, and on the other hand it is assumed that the heat fiux orthogonal to the applied gradient is zero, which always automatically sets the effective conductivity $k_{x y}^{*}$ to zero (compare equation (8)). Only for sufficiently large random unit cells with almost isotropic effective conductivities can this effect be neglected.

For the numerical and analytical studies, conductivities are chosen to be independent of the temperature. Nevertheless the studies can be readily extended to the case of temperature dependent conductivities by repeatedly running the calculations with the appropriate constituent conductivities corresponding to a particular temperature. With this procedure the temperature dependent thermal composite behaviour is predicted for discrete temperatures for small temperature differences within the unit cell.
It should be noted that only stationary fields are considered, i.e. initial temperature distributions, specific heat and constituent densities do not influence the effective conductivities of the composite. Investigations of transient processes seem feasible by means of appropriate FEM models, yielding time-dependent and local effective conductivities.

UNIT CELLS FOR STAGGERED SHORT FIBRE COMPOSITES


3 a different staggered and non-staggered arrangements of aligned short fibres (aspect ratio $=10$ ) for axial fibre offset $\alpha=0.25 ; b$ geometry parameters $\delta$ and $\alpha$ describe degree of staggering and axial fibre offset

## issue of boundary conditions EFFECTIVE CONDUCTIVITIES

For the numerical and analytical studies, conductivities are chosen to be independent of the temperature. Nevertheless the studies can be readily extended to the case of temperature dependent conductivities by repeatedly running the calculations with the appropriate constituent conductivities corresponding to a particular temperature. With this procedure the temperature dependent thermal composite behaviour is predicted for discrete temperatures for small temperature differences within the unit cell.
It should be noted that only stationary fields are considered, i.e. initial temperature distributions, specific heat and constituent densities do not influence the effective conductivities of the composite. Investigations of transient processes seem feasible by means of appropriate FEM models, yielding time-dependent and local effective conductivities.

## Results and discussion

As an example carbon/copper composites are chosen, which are produced by hot pressing; matrix and fibre material data are listed in Table 1. The conductivity of the isotropic copper matrix is approximately $10 \%$ less than the theoretical conductivity of $99 \%$ copper, due to contamination and pores left after the hot pressing process.

All calculations are carried out for carbon/copper composites with a fibre volume fraction $\check{\zeta}=0 \cdot 4$. The fibres in SFRCs are modelled as cylinders with an aspect ratio of 10 .
Unit cell calculations are carried out with the finite element program ANSYS 5.7. ${ }^{23}$ Two dimensional unit cells are meshed with six node triangular elements, three dimensional unit cells are meshed with 10 node tetrahedral elements. The thermal interface was modelled with appropriate contact/target surface elements, which are overlaid on the constituent interfaces, allowing for non-conformal meshes at the interface.
Thermal barrier interface The influence of the thermal interface is studied for a square and a rectangular ( $b-l$ $a_{\square}=0.6$ ) arrangement. The interface conductance ( $\beta \cdot r_{\text {fibre }}, r_{\text {fibre }}$ being the fibre radius) is varied from $10^{-3}$ to $10^{7} \mathrm{~W} \mathrm{~m}^{-1} \mathrm{~K}^{-1}$, covering the range from perfectly insulating interfaces to perfectly conducting interfaces.

## Failure of the end face interfaces

The influence of decohesion or lack of contact of the interfaces at the fibres' end faces, i.e. perfectly insulating interfaces, is also investigated. The effective axial conductivities are reduced severely while the effective transverse conductivity is less affected (Table 3, Fig. 6).

The effective transverse conductivity is reduced only slightly due to the presence of the thermal barrier at the end faces (for all arrangements the reduction is less than $0.1 \%$ ).
The setup of the microarrangements was highly idealised, as perfectly periodic arrangements are not fully realistic. Nevertheless useful insight and information on the interdependence of the topological input parameters was gained.

When compared to three dimensional unit cells with randomly oriented fibres, the cells employed for aligned fibres can be set up relatively easily to meet high fibre volume fractions requirements, and they are not very demanding with regard to computational requirements. The present approach can easily be applied to other microtopologies. Extensions to fully coupled thermomechanical investigations of high volume fraction, three dimensional unit cells with randomly oriented fibres and with consideration of load dependent progressive failure of the interfaces are feasible.

## INTRODUCTION (ix)

- Characteristics of composite materials
$>$ Presence of large number of particles or fibers.
$>$ Very disparate length scales:
$\checkmark$ MACROSCALE: physical dimension of the composite body ( $\mathrm{m} \rightarrow \mathrm{cm}$ );
$\checkmark$ MesoScale: characteristic dimension of the composite microstructure, RVE or cell ( $\mathrm{mm} \rightarrow \mu \mathrm{m}$ );
$\checkmark$ microscale: characteristic dimension of the particles/fibers ( $\mu \mathrm{m}$ ).
- Heat conduction in composites
$>$ Transport problem in multiple scale media.
$>$ Difficult direct application of conventional analytical and numerical methods.
$>$ Difficult determination of local temperature fields.
$>$ Macroscopic thermal behavior of a composite may be described, once the effective conductivity is known.


## BRIEF LITERATURE REVIEW (i)

- Bound methods
(Milton, 2002; Torquato, 1991; Nomura \& Chou, 1980)
$>$ Rigorous determination of lower and upper bounds.
$>$ General spatial correlation functions for the microstructure.
$>$ Do not agree well with experimental data when phase contrast (e.g., conductivity ratio) is high.
- Analytical and semi-analytical methods
(Cheng \& Torquato, 1997; Furmañski, 1991; Sangani \& Yao, 1988; Sangani \& Acrivos, 1983; Perrins et al., 1979)
$>$ Simple geometries (e.g., spheres, ellipsoids).
$>$ Dilute limit (low dispersed phase volume fractions).
$>$ May treat random distributions of particles.


## BRIEF LITERATURE REVIEW (ii)

- Phenomenological approaches
(Dunn et al., 1993; Hasselman et al., 1993; Benveniste et al., 1990; Hatta \& Taya, 1986; Hashin, 1968)
>Simplifying heuristic assumptions: mean field concept of Mori-Tanaka, equivalent inclusion method of Eshelby.
$>$ Distributions of orientation and aspect ratio of fibers.
$>$ Interactions of neighboring fibers are neglected.
$>$ Most works assume perfect thermal contact.
$>$ Expressions for the effective thermal conductivity "valid" for low to moderate dispersed phase volume fractions.


## BRIEF LITERATURE REVIEW (iii)

- Computational approaches
(Matt \& Cruz, 2006; Duschlbauer et al., 2003; Matt \& Cruz, 2002; Matt \& Cruz, 2001; Rocha \& Cruz, 2001; Ingber et al., 1994; Veyret et al., 1993; James \& Keen, 1985)
$>$ Flexibility to incorporate geometrical and physical effects.
$>$ Mostly restricted to 2-D microstructures.
$>$ Microstructure must be prescribed.
$>$ FEM, FDM, BEM.
$>$ So far, not systematically applied to 2-D and 3-D composites with realistic geometrical and physical features.


## BRIEF LITERATURE REVIEW (iv)

- Experimental measurements
(Jiajun \& Xiao-Su, 2004; Garnier et al., 2002; Mirmira \& Fletcher, 2001; Mirmira, 1999)
$>$ The truth: complete physics, hard to fully characterize.
> Criticism: majority of existing methodologies overestimate the effective thermal conductivity of composites.
$>$ Estimation of interfacial thermal resistance.
$>$ Estimation of volume fraction of pores inside the matrix.
$>$ Information about shape and orientation of fibers.
$>$ Still: difficult comparison with theoretical/numerical predictions.


## HEAT CONDUCTION IN COMPOSITES (i)

- Physical description

composite with 3-D microstructure


## HEAT CONDUCTION IN COMPOSITES (ii)

- Mathematical formulation, dimensional strong form



## HEAT CONDUCTION IN COMPOSITES (iii)

- Mathematical formulation, non-dimensional strong form

$$
\begin{aligned}
& -\frac{\partial}{\partial y_{i}}\left(\frac{\partial \theta^{m}}{\partial y_{i}}\right)=\frac{\dot{g}_{m} \lambda^{2}}{k^{m} \Delta T} \text { em } \Omega_{m} \\
& -\frac{\partial}{\partial y_{i}}\left(\kappa_{i j} \frac{\partial \theta^{d}}{\partial y_{j}}\right)=\frac{\dot{g}_{d} \lambda^{2}}{k_{k}^{m} \Delta T} \text { em } \Omega_{d} \\
& -\frac{\partial \theta^{m}}{\partial y_{i}} n_{i}^{m}=-\kappa_{i j} \frac{\partial \theta^{d}}{\partial y_{j}} n_{i}^{m} \text { em } \partial \Omega_{s} \\
& -\frac{\partial \theta^{m}}{\partial y_{i}} n_{i}^{m}=\frac{h_{\mathrm{s}} \lambda}{k^{m}}\left(\theta^{\square}-\theta^{d}\right) \text { em } \partial \Omega_{s} \\
& \rightarrow \begin{array}{l}
\text { magnitude of interfacial } \\
\text { thermal resistance }
\end{array}
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{y} & \equiv \frac{\mathbf{x}^{*}}{\lambda}, \\
\theta^{m}\left(\mathbf{x}^{*}\right) & \equiv \frac{T^{m}\left(\mathbf{x}^{*}\right)}{\Delta T} \\
\theta^{d}\left(\mathbf{x}^{*}\right) & \equiv \frac{T^{d}\left(\mathbf{x}^{*}\right)}{\Delta T} \\
k_{i j} & \equiv \frac{k_{i j}^{d}}{k^{m}} \\
G_{m} & \equiv \frac{\dot{g}_{m^{\prime}} \lambda^{2}}{k^{m} \Delta T} \\
G_{d} & \equiv \frac{\dot{g}_{d} \lambda^{2}}{k^{m} \Delta T} \\
\mathrm{Bi} & \equiv \frac{h_{\mathrm{s}} \lambda}{k^{m}}
\end{aligned}
$$

## HEAT CONDUCTION IN COMPOSITES (iv)

- Mathematical formulation, weak form
> Advantages of weak form
$\checkmark$ Boundary condition of continuity of heat flux at the interface is naturally imposed ( $\Rightarrow$ easy to incorporate voids).
$\checkmark$ Compatibility with the finite element method.
$>$ Definition of function spaces

$$
\begin{aligned}
X^{\prime}(\Omega)=\left\{w \in H^{1}(\Omega)|w| \Omega_{c} \subset \Omega=\right. & \left.w^{c}, w_{\Omega_{d} \subset \Omega}=w^{d},[w]_{\partial \Omega_{s}}=s \in \mathbb{R}\right\} \\
& X^{\prime}(\Omega) \text { allows jumps at the interface } \\
X(\Omega)=X^{\prime}(\Omega) \cap H_{0}^{1}(\Omega) \quad & H_{0}^{1}(\Omega) \subset H^{1}(\Omega)
\end{aligned}
$$

## HEAT CONDUCTION IN COMPOSITES (v)

- Mathematical formulation, weak form
$>$ Statement
given $\zeta_{i j}(\mathbf{y})$, Bi and $G(\mathbf{y})$, find $\theta(\mathbf{y}) \in X^{\prime}(\Omega)$ such that

$$
\begin{gathered}
\int_{\Omega} \zeta_{i j}(\mathbf{y}) \frac{\partial \theta}{\partial y_{j}} \frac{\partial v}{\partial y_{i}} d \mathbf{y}+\int_{\partial \Omega_{s}} \operatorname{Bi}[v]_{\partial \Omega_{s}}[\theta]_{\partial \Omega_{s}} d s=\int_{\Omega} v G d \mathbf{y} \quad \forall v \in X(\Omega) \\
v, \theta, \zeta_{i j}(\mathbf{y}), G= \begin{cases}v^{m}, \theta^{m}, \delta_{i j}, G_{m} & \text { in } \quad \Omega_{m} \subset \Omega \\
v^{d}, \theta^{d}, \kappa_{i j}, G_{d} & \text { in } \quad \Omega_{d} \subset \Omega .\end{cases}
\end{gathered}
$$

## HEAT CONDUCTION IN COMPOSITES (vi)

- Homogenization theory
(Milton, 2002; Auriault \& Ene, 1994; Auriault, 1991; Bakhvalov \& Panasenko, 1989; Bensoussan et al., 1978; Babuska, 1975)
$>$ Rigorous mathematical technique.
$>$ Applied to a variety of transport phenomena in heterogeneous media.
$>$ Exact solution behavior in the limit that the ratio of length scales tends to zero.
$>$ Transforms the transport problem defined in the original heterogeneous medium in two easier problems to solve:
$\checkmark$ homogenized problem;
$\checkmark$ cell problem.


## HEAT CONDUCTION IN COMPOSITES (vii)

- Homogenization theory

Schematic illustration of the method

heterogeneous medium
homogeneous medium

## HEAT CONDUCTION IN COMPOSITES (viii)

- Homogenization theory

Technique of asymptotic expansions using multiple scales
$>$ Appropriate for transport problems defined in statistically homogeneous media that exhibit a natural separation of length scales: $\epsilon \equiv \lambda / L \ll 1$.
$>$ Solution is written as a function of two variables:
$\checkmark$ fast variable (mesoscale coordinate);
$\checkmark$ slow variable (macroscale coordinate).

$$
\begin{aligned}
\theta(\mathrm{x}, \mathrm{y}) & =\theta_{0}(\mathrm{x}, \mathrm{y})+\epsilon \theta_{1}(\mathrm{x}, \mathrm{y})+\epsilon^{2} \theta_{2}(\mathrm{x}, \mathrm{y})+\ldots \\
v(\mathrm{x}, \mathrm{y}) & =v_{0}(\mathrm{x}, \mathrm{y})+\epsilon v_{1}(\mathrm{x}, \mathrm{y})+\epsilon^{2} v_{2}(\mathrm{x}, \mathrm{y})+\ldots
\end{aligned}
$$

$$
\mathrm{y} \equiv \mathrm{x}^{*} / \lambda
$$

(fast variable )

$$
\mathrm{x} \equiv \mathrm{x}^{*} / L=\epsilon \mathbf{y}
$$

(slow variable )

## HEAT CONDUCTION IN COMPOSITES (ix)

## - Application of the method

$>$ Substituting the expansions for $\theta$ and $v$ in the weak form...

$$
\begin{aligned}
& \int_{\Omega} \zeta_{i j}\left(\frac{\partial v_{0}}{\partial y_{i}}+\epsilon \frac{\partial v_{0}}{\partial x_{i}}+\epsilon \frac{\partial v_{1}}{\partial y_{i}} \epsilon^{2} \frac{\partial v_{1}}{\partial x_{i}}+\epsilon^{2} \frac{\partial v_{2}}{\partial y_{i}}\right)\left(\frac{\partial \theta_{0}}{\partial y_{j}}+\epsilon \frac{\partial \theta_{0}}{\partial x_{j}}+\epsilon \frac{\partial \theta_{1}}{\partial y_{j}}+\epsilon^{2} \frac{\partial \theta_{1}}{\partial x_{j}}+\epsilon^{2} \frac{\partial \theta_{2}}{\partial y_{j}}\right) d y \\
& +\int_{\partial \Omega_{s}} \mathrm{Bi}\left[v_{0}+\epsilon v_{1}+\epsilon^{2} v_{2}\right]_{\Omega_{s},}\left[\theta_{0}+\epsilon \theta_{1}+\epsilon^{2} \theta_{2}\right]_{\partial \Omega_{s}} d \mathrm{~s} \\
& =\int_{\Omega}\left(v_{0}+\epsilon v_{1}+\epsilon^{2} v_{2}\right) G d y \forall v_{v}, v_{1}, v_{2} \in X(\Omega)
\end{aligned}
$$

$>$ Homogenization condition: $\quad \theta_{0} \neq 0 \quad \Rightarrow \quad G=O\left(\epsilon^{2}\right)$
(the heat generated internally to the composite must have the same order of magnitude of the heat conducted on the macroscale)
$>$ Five models, depending on the magnitude of the interfacial thermal resistance (Rocha \& Cruz, 2001; Auriault \& Ene, 1994)

$$
\mathrm{Bi}=O\left(\epsilon^{a}\right), a \in\{-1,0,1,2,3\} \quad \text { Here: Model II, } a=0 .
$$

## HEAT CONDUCTION IN COMPOSITES (x)

- Application of the method
$>$ Grouping equal powers of $\varepsilon$...

$$
\begin{aligned}
& {\left[\theta_{0}^{\mathrm{II}}\right]_{\partial \Omega_{s}}=0} \\
& \frac{\partial \theta_{0}^{\mathrm{II}}}{\partial y_{j}}=0, j=1,2,3 \\
& \int_{\Omega} \zeta_{i j}\left(\frac{\partial \theta_{0}^{17}}{\partial x_{j}} \frac{\partial v_{0}^{17}}{\partial x_{i}}+\frac{\partial \theta_{1}^{1]}}{\partial y_{j}} \frac{\partial v_{0}^{I I}}{\partial x_{i}}+\frac{\partial \theta_{0}^{17}}{\partial x_{j}} \frac{\partial v_{1}^{11}}{\partial y_{i}}+\frac{\partial \theta_{1}^{11}}{\partial y_{j}} \frac{\partial v_{1}^{11}}{\partial y_{i}}\right) d y+ \\
& +\int_{\partial \Omega_{s}} \operatorname{Bi}\left[v_{1}^{1]_{\partial \Omega_{s}}}{ }_{\partial 1}\left[\theta_{1}^{\mathrm{T}}\right]_{\partial n_{s}} d s=\int_{\Omega} v_{0}^{11} G d y\right. \\
& \forall v_{0}^{\mathrm{II}}, v_{1}^{\mathrm{II}} \in X(\Omega)
\end{aligned}
$$

## HEAT CONDUCTION IN COMPOSITES (xi)

- Application of the method $>$ Choosing, first, $v_{0}{ }^{\mathrm{II}}=0$ and, next, $v_{1}{ }^{\mathrm{II}}=0 \ldots$

$$
\begin{aligned}
& v_{0}^{\mathrm{II}}=0 \\
& \int_{\Omega} \zeta_{i j} \frac{\partial v_{1}^{\mathrm{II}}}{\partial y_{i}}\left(\frac{\partial \theta_{0}^{\mathrm{II}}}{\partial x_{j}}+\frac{\partial \theta_{1}^{\mathrm{II}}}{\partial y_{j}}\right) d \mathbf{y}+\int_{\partial \Omega_{s}} \operatorname{Bi}\left[v_{1}^{\mathrm{II}}\right]_{\partial \Omega_{s}}\left[\theta_{1}^{\mathrm{II}}\right]_{\partial \Omega_{s}} d s=0 \quad \forall v_{1}^{\mathrm{II}} \in X(\Omega) \\
& v_{1}^{\mathrm{II}}=0 \\
& \int_{\Omega} \zeta_{i j} \frac{\partial v_{0}^{\mathrm{II}}}{\partial x_{i}}\left(\frac{\partial \theta_{0}^{\mathrm{II}}}{\partial x_{j}}+\frac{\partial \theta_{1}^{\mathrm{II}}}{\partial y_{j}}\right) d \mathbf{y}=\int_{\Omega} v_{0}^{\mathrm{II}} G d \mathbf{y} \quad \forall v_{0}^{\mathrm{II}} \in X(\Omega)
\end{aligned}
$$

## HEAT CONDUCTION IN COMPOSITES (xii)

- Application of the method
$>$ Assuming separation of variables for $\theta_{1}{ }^{\mathrm{II}}(\mathbf{x}, \mathbf{y}) \ldots$

$$
\theta_{1}^{\mathrm{T1}^{1}}(\mathrm{x}, \mathrm{y})=-\chi_{p}^{\mathrm{II}_{p}}(\mathrm{y}) \frac{\partial \theta_{0}^{\mathrm{Ti}^{1}}}{\partial x_{p}}(\mathrm{x})
$$

> Applying the periodicity property to the volume integrals (Auriault, 1991; Rocha \& Cruz, 2001) and surface integrals (Rocha \& Cruz, 2001)...

$$
\lim _{\epsilon \rightarrow 0}\left(\int_{\Omega} f(\mathbf{x}, \mathbf{y}) d \mathbf{y}+\int_{\Omega \Omega_{s}} g(\mathbf{x}, \mathbf{y}) d s\right)=\int_{\Omega} \frac{1}{\left|\Omega_{p c}\right|}\left(\int_{\Omega_{0 c}} f(\mathbf{x}, \mathbf{y}) d \mathbf{y}+\int_{\Gamma} g(\mathbf{x}, \mathbf{y}) d s\right) d \mathbf{y}
$$

$\Omega_{p c} \quad$ representative volume element (RVE) of microstructure (assumed periodic) or periodic cell
$\Gamma$ portion of phase interface inside $\Omega_{\mathrm{pc}}$

## HEAT CONDUCTION IN COMPOSITES (xiii)

- Results of the method
$>$ Cell problem

$$
\begin{aligned}
& \int_{\Omega_{p c}} \zeta_{i j} \frac{\partial \chi_{p}^{\mathrm{II}}}{\partial y_{j}} \frac{\partial v}{\partial y_{j}} d \mathbf{y}+\int_{\Gamma} \operatorname{Bi}[v]_{\Gamma}\left[\chi_{p}^{\mathrm{II}}\right]_{\Gamma} d s=\int_{\Omega_{p c}} \zeta_{i p} \frac{\partial v}{\partial y_{i}} d \mathbf{y} \quad \forall v \in Y^{\mathrm{II}}\left(\Omega_{p c}\right) \\
& Y^{\mathrm{II}}\left(\Omega_{p c}\right)=\left\{w \in H_{\#}^{1}\left(\Omega_{p c}\right) \mid w_{\Omega_{p c}, c} \subset \Omega_{p c}=w^{c}, w_{\Omega_{p, d} \subset \subset \Omega_{p c}}=w^{d},[w]_{\Gamma}=s \in R^{*}\right\}
\end{aligned}
$$

$>$ Homogenized problem
> Effective thermal conductivity tensor

$$
\kappa_{p q}^{\epsilon, \mathrm{II}} \equiv \frac{k_{p q}^{\epsilon, \mathrm{II}}}{k^{m}}=\frac{1}{\left|\Omega_{p c}\right|} \int_{\Omega_{p c}} \zeta_{p i}\left(\delta_{i q}-\frac{\partial \chi_{q}^{\mathrm{II}}}{\partial y_{i}}\right) d \mathbf{y}
$$

## NUMERICAL METHODS (i)

- Geometrical models for the periodic cell
$>$ Ordered arrays of spheres

$>$ Disordered arrays of spheres

multi-particle cells



## NUMERICAL METHODS (ii)

- Geometrical models for the periodic cell
$>$ Ordered and disordered arrays of cylinders



## NUMERICAL METHODS (iii)

- Mesh generation in 3-D

Procedure uses generator NETGEN (Schöberl, 2002)


$$
c=0,50
$$


$c=0,30$
$\rho=0,5$

## NUMERICAL METHODS (iv)

- Mesh generation in 3-D Procedure uses generator NETGEN (Schöberl, 2002)

$$
c=0,75 \quad c=0.15
$$

$$
\rho_{p}=\rho_{f}=5
$$

## NUMERICAL METHODS (v)

- Finite element discretization
$>$ First order isoparametric
$\checkmark$ Solution and geometry interpolated by 10 degree polynomials.
$\checkmark$ Simple computational implementation.
$\checkmark$ Volume and surface integrals can be evaluated analytically.
$\checkmark$ Quadratic convergence of $k_{e, i j}$.
$\checkmark$ Accurate results for $k_{e, i j}>100$ only with excessive refinement of the mesh, a burden on computational time.


## NUMERICAL METHODS (vi)

- Finite element discretization
$>$ Second order isoparametric
$\checkmark$ Solution and geometry interpolated by $2 \underline{0}$ degree polynomials.
$\checkmark$ More sophisticated computational implementation.
$\checkmark$ Volume and surface integrals must be evaluated numerically.
$\checkmark$ Cubic convergence of $k_{e, i j}$.
$\checkmark$ Accurate results for $k_{e, i j}>100$ without the need for an excessive refinement of the mesh.


## NUMERICAL METHODS (vii)

- Finite element discretization


## $>$ Cell problem

$$
\begin{gathered}
a\left(v, \chi_{p}^{\mathrm{II}}\right)+b_{\Gamma}\left(v, \chi_{p}^{\mathrm{II}}\right)=\ell(v) \quad \forall v \in Y^{\mathrm{II}}\left(\Omega_{p c}\right) \\
a\left(v, \chi_{p}^{\mathrm{II}}\right)=\int_{\Omega_{p c}} \zeta_{i j}(\mathbf{y}) \frac{\partial \chi_{p}^{\mathrm{II}}}{\partial y_{j}} \frac{\partial v}{\partial y_{i}} d \mathbf{y} \quad \begin{array}{l}
\text { bilinear operator, symmetric and positive- } \\
\text { definite }
\end{array} \\
\ell(v)=\int_{\Omega_{p c}} \zeta_{i p}(\mathbf{y}) \frac{\partial v}{\partial y_{i}} d \mathbf{y} \quad \begin{array}{l}
\text { linear functional related to direction of temperature } \\
\text { gradient imposed externally }
\end{array} \\
b_{\Gamma}\left(v, \chi_{p}^{\mathrm{II}}\right)=\int_{\Gamma} \mathrm{Bi}\left[\chi_{p}^{\mathrm{II}}\right]_{\Gamma}[v]_{\Gamma} d \mathbf{s} \quad \text { bilinear and symmetric operator }
\end{gathered}
$$

## NUMERICAL METHODS (viii)

- Finite element discretization
> Treatment of volume integrals
Galerkin Method (Reddy, 1993; Hughes, 1987)

$$
\chi_{p}^{\epsilon} \equiv \chi_{p}^{\mathrm{II}} \mid \Omega_{\Omega^{e}}=\sum_{a=1}^{10} \chi_{p, a}^{\epsilon} \psi_{a}^{\epsilon}
$$

$\square$

$$
\left.v^{e} \equiv v\right|_{\Omega^{e}}=\sum_{b=1}^{10} v_{b}^{e} \psi_{b}^{e}
$$

$f_{a}^{\epsilon}=\int_{\Omega^{e}} \zeta_{i p}^{\epsilon} \frac{\partial \psi_{a}^{e}}{\partial y_{i}} d \mathbf{y}=\int_{0}^{1} \int_{0}^{1-\xi} \int_{0}^{1-\xi-\eta} \zeta_{i p}^{\epsilon}\left(\frac{\partial \psi_{a}^{e}}{\partial \xi} \frac{\partial \xi}{\partial y_{i}}+\frac{\partial \psi_{a}^{e}}{\partial \eta} \frac{\partial \eta}{\partial y_{i}}+\frac{\partial \psi_{a}^{e}}{\partial \zeta} \frac{\partial \zeta}{\partial y_{i}}\right) \operatorname{det} \mathbf{J}^{\epsilon} d \zeta d \eta d \xi$
$k_{a b}^{e}=\int_{\Omega^{e}} \zeta_{i j}^{e} \frac{\partial \psi_{a}^{e}}{\partial y_{j}} \frac{\partial \psi_{b}^{e}}{\partial y_{i}} d \mathbf{y}$
$=\int_{0}^{1} \int_{0}^{1-\xi} \int_{0}^{1-\xi-\eta} \zeta_{i j}^{e}\left(\frac{\partial \psi_{a}^{e}}{\partial \xi} \frac{\partial \xi}{\partial y_{j}}+\frac{\partial \psi_{a}^{e}}{\partial \eta} \frac{\partial \eta}{\partial y_{j}}+\frac{\partial \psi_{a}^{e}}{\partial \zeta} \frac{\partial \zeta}{\partial y_{j}}\right)\left(\frac{\partial \psi_{b}^{e}}{\partial \xi} \frac{\partial \xi}{\partial y_{j}}+\frac{\partial \psi_{b}^{e}}{\partial \eta} \frac{\partial \eta}{\partial y_{j}}+\frac{\partial \psi_{b}^{e}}{\partial \zeta} \frac{\partial \zeta}{\partial y_{j}}\right) \operatorname{det} \mathbf{J}^{e} d \zeta d \eta d \xi$

## NUMERICAL METHODS (ix)

- Finite element discretization
> Treatment of surface integral
$\checkmark$ Duplication of degrees of freedom associated with global nodes situated on the interface $\Gamma$
$\checkmark$ Modification of tetrahedra connectivity that possess at least one node on $\Gamma$
$\checkmark$ Calculation of the jumps of the functions (weight, test) through the element surfaces on $\Gamma$
$\checkmark$ Integration of the product of the jumps in $\Gamma$
$\checkmark$ Sum of the resulting integrals to the appropriate components in the global stiffness matrix


## Duplication of degrees of freedom and Modification of tetrahedra connectivity

## BEFORE DUPLICATION



## AFTER DUPLICATION



## NUMERICAL METHODS (x)

- Contributions associated with node of vertex $A$
$>$ Weight function restricted to node $A$

$$
\left.v_{A}\right|_{e, \Gamma}=\left.\phi_{A}^{c}\right|_{e, \Gamma}
$$

$>$ Jump of weight function across $\Gamma_{\mathrm{ee}}$,

$$
\left[v_{A}\right]_{e_{e \prime}}=\left.v_{A}\right|_{e, \Gamma}-\overbrace{\left.v_{A}\right|_{e, \Gamma}}^{0}=\left.v_{A}\right|_{e, \Gamma}=\left.\phi_{A}^{c}\right|_{e, \Gamma}
$$

$>$ Jump of temperature across $\Gamma_{\mathrm{ee}}$,

$$
\begin{aligned}
& {\left[\chi_{p, h}^{\mathrm{II}}\right]_{\Gamma_{e e^{\prime}}}=\left.\chi_{A} \phi_{A}^{c}\right|_{e, \Gamma}+\left.\chi_{B} \phi_{B}^{c}\right|_{e, \Gamma}+\left.\chi_{C} \phi_{C}^{c}\right|_{e, \Gamma}+\left.\chi_{M} \phi_{M}^{c}\right|_{e, \Gamma}+\left.\chi_{N} \phi_{N}^{c}\right|_{e, \Gamma}+\left.\chi_{P} \phi_{P}^{c}\right|_{e, \Gamma}-} \\
& \left.\chi_{A^{\prime}} \phi_{A^{\prime}}^{d}\right|_{e^{\prime}, \Gamma}-\left.\chi_{B^{\prime}} \phi_{B^{\prime}}^{d}\right|_{e^{\prime}, \Gamma}-\left.\chi_{C^{\prime}} \phi_{C^{\prime}}^{d}\right|_{e^{\prime}, \Gamma}-\left.\chi_{M^{\prime}} \phi_{M^{\prime}}^{d}\right|_{e^{\prime}, \Gamma}-\left.\chi_{N^{\prime}} \phi_{N^{\prime}}^{d}\right|_{e^{\prime}, \Gamma}-\left.\chi_{P^{\prime}} \phi_{P^{\prime}}^{d}\right|_{e^{\prime}, \Gamma}
\end{aligned}
$$

## NUMERICAL METHODS (xi)

- Contributions associated with node of vertex $A$

$$
\begin{aligned}
& \text { sum to component } K_{A A} \\
& \int_{\Gamma_{e e^{\prime}}} \operatorname{Bi}\left[v_{A}\right]_{\Gamma_{e e^{\prime}}}\left[\chi_{p, h}^{\mathrm{II}}\right]_{\Gamma_{e e^{\prime}}} d \mathbf{s}=\operatorname{Bi}\left(\chi_{A} \sqrt{\left.\left.\int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{A}^{c}\right|_{e, \Gamma} d \mathbf{s}}+\left.\left.\chi_{B} \int_{\Gamma_{e e^{\prime}}} \phi_{A, \Gamma}^{c}\right|_{e, \Gamma} \phi_{B}^{c}\right|_{e, \Gamma} d \mathbf{s}+\right. \\
& \left.\left.\chi_{C} \int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{C}^{c}\right|_{e, \Gamma} d \mathbf{s}+\left.\left.\chi_{M} \int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{M}^{c}\right|_{e, \Gamma} d \mathbf{s}+\left.\left.\chi_{N} \int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{N}^{c}\right|_{e, \Gamma} d \mathbf{s}+ \\
& \left.\left.\chi_{P} \int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{P}^{c}\right|_{e, \Gamma} d \mathbf{s}-\left.\left.\chi_{A^{\prime}} \int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{A^{\prime}}^{d}\right|_{e^{\prime}, \Gamma} d \mathbf{s}-\left.\left.\chi_{B^{\prime}} \int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{B^{\prime}}^{d}\right|_{e^{\prime}, \Gamma} d \mathbf{s}- \\
& \left.\left.\chi_{C^{\prime}} \int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{C^{\prime}}^{d}\right|_{e^{\prime}, \Gamma} d \mathbf{s}-\left.\left.\chi_{M^{\prime}} \int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{M^{\prime}}^{d}\right|_{e^{\prime}, \Gamma} d \mathbf{s}-\left.\left.\chi_{N^{\prime}} \int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{N^{\prime}}^{d}\right|_{e^{\prime}, \Gamma} d \mathbf{s}- \\
& \left.\left.\left.\chi_{P^{\prime}} \int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{P^{\prime}}^{d}\right|_{e^{\prime}, \Gamma} d \mathbf{s}\right)
\end{aligned}
$$

## NUMERICAL METHODS (xii)

- Algorithm

For each node situated on $\Gamma$
$>$ Identification of neighboring nodes (corner and median)
$>$ Identification of its duplicates and of duplicates of neighboring nodes
$>$ Definition of weight function restricted to node and tetrahedra which share the node on $\Gamma$
$>$ Calculation of jumps of weight and temperature functions across tetrahedra surfaces which share the node on $\Gamma$
$>$ Evaluation of resulting integrals
$>$ Sum of resulting integrals to the appropriate components in the global stiffness matrix

## NUMERICAL METHODS (xiii)

- Discrete system of equations

$$
\mathcal{K}^{*} \boldsymbol{\chi}_{p, h}^{\mathrm{II}}=\mathcal{F}^{*}
$$

Global stiffness matrix and global forcing vector assembled from elemental matrices and elemental vectors, imposing periodic boundary conditions on the outer surfaces of $\Omega_{p c}$

## NUMERICAL METHODS (xiv)

- Iterative method (global minimum residual, GMRES, Paige \& Saunders, 1975)
> Appropriate for linear systems of equations whose coefficient matrices are symmetric, but not necessarily positive-definite
$>$ Stopping criterion: based on the norm $L_{2}$ of the residual vector, subject to a user-prescribed tolerance $\sigma$

$$
\mathbf{A} \mathbf{u}=\mathbf{b}
$$

$$
\begin{aligned}
& \mathbf{r} \equiv \mathbf{b}-\mathbf{A} \mathbf{u}^{*} \mathbf{r}_{0} \equiv \mathbf{b}-\mathbf{A} \mathbf{u}^{*(0)} \\
&\|\mathbf{r}\|_{L_{2}}=\left(\mathbf{r}^{T} \mathbf{r}\right)^{1 / 2}\left\|\mathbf{r}_{0}\right\|_{L_{2}}=\left(\mathbf{r}_{0}^{T} \mathbf{r}_{0}\right)^{1 / 2} \\
& \frac{\|\mathbf{r}\|_{L_{2}}}{\left\|\mathbf{r}_{0}\right\|_{L_{2}}}<\sigma^{2}
\end{aligned}
$$

## RESULTS (i)

- 2-D effort: smaller than the 3-D effort, and it is (still) valuable for random arrangements
- Simple cubic array of spheres with uniform interfacial thermal resistance (and, also, with perfect thermal contact)
- Disordered array of spheres with uniform interfacial thermal resistance and pores in the matrix (illustrative computations)
- Parallelepipedonal array of cylinders with uniform interfacial thermal resistance
- Tentative comparison with experimental data
DETERMINAÇÃO DA CONDUTIVIDADE TÉRMICA EFETIVA DE
COMPÓSITOS FIBROSOS UNIDIRECIONAIS RANDÔMICOS


Figura 6.8: A célula de Voronoi com 17 fibras e $c=0,375$.

Table 1: Effective conductivity results for the square array
Parameters: $c \in\{0.75,0.78,0.785, \pi / 4\}, \alpha \in\{2,10,50\}$, $\beta \in\{0.04,0.06\}$.


## Extension

to 3-D

## ABSTRACT SUBMISSION

Authors should submit two copies of an abstract of approximately 500 words. Authors and co-authors are requested to provide their complete addresses, phone and fax numbers, and e -mail addresses.

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## Simple cubic array of spheres

Validation with semi-analytical results by Cheng \& Torquato (1997)

$$
R_{c}=\kappa-1
$$

critical thermal contact resistance

| $c$ | $\alpha=10, R_{c}=9$ |  |  |  | $\alpha=10000, R_{c}=9999$ |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $R=5$ |  | $R=30$ |  | $R=5000$ |  | $R=20000$ |  |
|  | $\kappa_{e}^{h}$ | $\kappa_{e}^{\mathrm{CT}}$ | $\kappa_{e}^{h}$ | $\kappa_{e}^{\mathrm{CT}}$ | $\kappa_{e}^{h}$ | $\kappa_{e}^{\mathrm{CT}}$ | $\kappa_{e}^{h}$ | $\kappa_{e}^{\mathrm{CT}}$ |
| 0,05 | 1,0275 | 1,0275 | 0,9569 | 0,9569 | 1,0379 | 1,0380 | 0,9703 | 0,9703 |
| 0,10 | 1,0556 | 1,0556 | 0,9150 | 0,9150 | 1,0768 | 1,0769 | 0,9412 | 0,9412 |
| 0,15 | 1,0841 | 1,0841 | 0,8742 | 0,8742 | 1,1168 | 1,1168 | 0,9126 | 0,9126 |
| 0,20 | 1,1131 | 1,1132 | 0,8348 | 0,8348 | 1,1577 | 1,1578 | 0,8845 | 0,8845 |
| 0,25 | 1,1428 | 1,1428 | 0,7957 | 0,7957 | 1,1997 | 1,1998 | 0,8569 | 0,8569 |
| 0,30 | 1,1728 | 1,1729 | 0,7577 | 0,7577 | 1,2428 | 1,2429 | 0,8299 | 0,8298 |
| 0,35 | 1,2036 | 1,2036 | 0,7203 | 0,7203 | 1,2870 | 1,2870 | 0,8030 | 0,8029 |
| 0,40 | 1,2346 | 1,2347 | 0,6834 | 0,6833 | 1,3321 | 1,3322 | 0,7764 | 0,7763 |
| 0,45 | 1,2663 | 1,2663 | 0,6465 | 0,6464 | 1,3783 | 1,3783 | 0,7499 | 0,7498 |
| 0,50 | 1,2983 | 1,2983 | 0,6092 | 0,6091 | 1,4255 | 1,4254 | 0,7234 | 0,7232 |
| 0,51 | 1,3047 | 1,3047 | 0,6016 | 0,6015 | 1,4349 | 1,4349 | 0,7180 | 0,7178 |

Simple cubic array of spheres with uniform interfacial thermal resistance Validation with semi-analytical results by Cheng \& Torquato (1997) Convergence plots of absolute error


## Simple cubic array of spheres

Distinct behaviors for the effective thermal conductivity as a function of the magnitude of the interfacial thermal resistance


Disordered array of spheres with uniform interfacial thermal resistance and pores within the matrix (illustrative calculations, acurate: novelty!)

| Values of $k_{e}^{\mathrm{N}}(\mathcal{C})$ for $c=0.15$ |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
| $\alpha=10$ |  |  |  |  |
| $R_{c}=9$ |  |  |  |  |
| Without voids |  |  |  |  |
| $\mathcal{C}$ | $R=5$ | $R=30$ | $R=5$ | $R=30$ |
| 1 | 1.0286 | 0.8509 | 1.0256 | 0.8469 |
| 2 | 1.0284 | 0.8466 | 1.0250 | 0.8440 |
| 3 | 1.0288 | 0.8571 | 1.0254 | 0.8543 |
| 4 | 1.0286 | 0.8518 | 1.0253 | 0.8490 |
| 5 | 1.0287 | 0.8557 | 1.0257 | 0.8525 |
| 6 | 1.0287 | 0.8535 | 1.0255 | 0.8502 |
| 7 | 1.0284 | 0.8462 | 1.0252 | 0.8424 |
| 8 | 1.0287 | 0.8548 | 1.0256 | 0.8502 |
| 9 | 1.0282 | 0.8409 | 1.0251 | 0.8371 |
| 10 | 1.0280 | 0.8337 | 1.0248 | 0.8305 |
| $k_{e}^{\mathrm{N}}$ | 1.0285 | 0.849 | 1.0253 | 0.846 |
| $S_{k_{e}^{\mathrm{N}}}$ | 0.0003 | 0.007 | 0.0003 | 0.007 |
| $k_{e}^{\mathrm{B}}$ | 1.0308 | 0.851 | - | - |


| Values of $k_{e}^{\mathrm{N}}(\mathcal{C})$ for $c=0.15$ |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $\alpha=10000, R_{c}=9999$ |  |  |  |  |  |
| Without voids |  |  |  | With $0.56 \%$ voids |  |
| $\mathcal{C}$ | $R=5000$ | $R=20000$ | $R=5000$ | $R=20000$ |  |
| 1 | 1.0497 | 0.8789 | 1.0469 | 0.8751 |  |
| 2 | 1.0492 | 0.8761 | 1.0457 | 0.8733 |  |
| 3 | 1.0505 | 0.8831 | 1.0470 | 0.8802 |  |
| 4 | 1.0498 | 0.8795 | 1.0465 | 0.8766 |  |
| 5 | 1.0503 | 0.8821 | 1.0472 | 0.8790 |  |
| 6 | 1.0500 | 0.8807 | 1.0469 | 0.8774 |  |
| 7 | 1.0492 | 0.8758 | 1.0460 | 0.8721 |  |
| 8 | 1.0502 | 0.8816 | 1.0473 | 0.8772 |  |
| 9 | 1.0487 | 0.8724 | 1.0457 | 0.8688 |  |
| 10 | 1.0480 | 0.8678 | 1.0448 | 0.8646 |  |
| $k_{e}^{\mathrm{N}}$ | 1.0496 | 0.878 | 1.0464 | 0.874 |  |
| $S_{k_{\mathrm{e}}^{\mathrm{N}}}$ | 0.0008 | 0.005 | 0.0008 | 0.005 |  |
| $k_{e}^{\mathrm{B}}$ | 1.0522 | 0.880 | - | - |  |

Parallelepipedonal array of cylinders
Validation with rule-of-mixtures results, and results from the expression by Hasselman \& Johnson (1987) for unidirectional fibrous composites with low $c$

| $c=0,10, \rho_{p}=5 \mathrm{e} \alpha=100$ |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\rho_{f}$ | $\mathrm{Bi}=10^{-6}$ |  | $\mathrm{Bi}=10^{-1}$ |  | $\mathrm{Bi}=10^{2}$ |  |
|  | $\kappa_{11}^{e, h}$ | $\kappa_{22}^{e, h}$ | $\kappa_{11}^{e, h}$ | $\kappa_{22}^{e, h}$ | $\kappa_{11}^{e, h}$ | $\kappa_{22}^{e, h}$ |
| 6 | 0,8852 | 0,8335 | 0,9619 | 0,8401 | 1,9352 | 1,2283 |
| 8 | 0,8902 | 0,8286 | 0,9991 | 0,8349 | 2,3972 | 1,2160 |
| 12 | 0,8956 | 0,8226 | 1,0839 | 0,8285 | 4,1371 | 1,2023 |
| 13,5 | 0,8981 | 0,8204 | 1,1214 | 0,8262 | 5,8827 | 1,1964 |
| $\rho_{t, \max }=14$ | 10,900 | 0,8182 | 10,900 | 0,8240 | 10,900 | 1,1920 |
|  | $\kappa_{e, \mathrm{~L}}^{\mathrm{RM}}$ | $\kappa_{e, T}^{\mathrm{H}}$ | $\kappa_{e, \mathrm{~L}}^{\mathrm{RM}}$ | $\kappa_{e, T}^{\mathrm{H}}$ | $\kappa_{e, \mathrm{~L}}^{\mathrm{RM}}$ | $\kappa_{e, T}^{\mathrm{H}}$ |
|  | 10,900 | 0,8182 | 10,900 | 0,8240 | 10,900 | 1,1920 |

## Parallelepipedonal array of cylinders

Sample of new results

Parallelepipedonal array $\rho_{p}=\rho_{f}=20$

| c | $\alpha=10$ |  |  |  | $\alpha=1000$ |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $\mathrm{Bi}=10^{-6}$ |  | $\mathrm{Bi}=10^{4}$ |  | $\mathrm{Bi}=10^{-6}$ |  | $\mathrm{Bi}=10^{4}$ |  |
|  | $\kappa_{11}^{e, h}$ | $\kappa_{22}^{e, h}$ | $\kappa_{11}^{e, h}$ | $\kappa_{22}^{e, h}$ | $\kappa_{11}^{e, h}$ | $\kappa_{22}^{e, h}$ | $\kappa_{11}^{e, h}$ | $\kappa_{22}^{e, h}$ |
| 0,10 | 0,8872 | 0,8356 | 1,4647 | 1,2005 | 0,8872 | 0,8356 | 1,9586 | 1,2586 |
| 0,20 | 0,7710 | 0,6971 | 1,8674 | 1,4490 | 0,7710 | 0,6971 | 2,6674 | 1,5990 |
| 0,30 | 0,6584 | 0,5743 | 2,3184 | 1,7568 | 0,6584 | 0,5743 | 3,5628 | 2,0540 |
| 0,40 | 0,5520 | 0,4613 | 2,8671 | 2,1432 | 0,5520 | 0,4613 | 4,8528 | 2,6847 |
| 0,50 | 0,4530 | 0,3541 | 3,5772 | 2,6441 | 0,453 | 0,354 | 6,977 | 3,627 |
| 0,60 | 0,3619 | 0,2492 | 4,5568 | 3,3292 | 0,362 | 0,249 | 11,27 | 5,244 |
| 0,70 | 0,2785 | 0,1406 | 6,0220 | 4,3667 | 0,278 | 0,141 | 25,03 | 9,094 |

## COMPARISON WITH EXPERIMENTAL DATA (tentative)

- Experimental work by Mirmira (1999)
$>$ Measurements of longitudinal and transverse effective thermal conductivities of short fiber composites as a function of temperature
> Characteristics of composites
$\checkmark$ Matrix: cianate ester
$\checkmark$ Dispersed phase: carbon fibers (DKE X, DKA X, K22XX)
$\checkmark$ Fiber volume fractions in fabricated composites: $55 \%, 65 \%$ and $75 \%$
$\checkmark$ Aspect ratio of fibers: 20
$\checkmark$ Pores volume fraction: $4 \%$ (estimation)
$\checkmark$ Estimated interfacial thermal conductance: $10^{5} \mathrm{~W} / \mathrm{m}^{2} \mathrm{~K}$
$\checkmark$ Fibers are distributed in parallel planes and randomly oriented


## COMPARISON WITH EXPERIMENTAL DATA (tentative)

- Numerical results: application of developed methodology to the parallelepipedonal array of cylinders
- Analytical results: expressions for the effective conductivities obtained by various authors for arrays of cylindrical fibers randomly arranged in space


## COMPARISON WITH EXPERIMENTAL DATA (tentative)

Symbols: Exp. $=$ experimental Num. $=$ numerical Analít. $=$ analytical (Dunn et al., 1993)

Composites with DKA X type fibers (longitudinal conductivity)

| T (K) | $55 \%$ |  |  | $65 \%$ |  |  | $75 \%$ |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Exp. | Num. | Analít. | Exp. | Num. | Analít. | Exp. | Num. | Analit. |
| 293,15 | 50,12 | 64,37 | 69,44 | 66,58 | 29,73 | 101,06 | 71,15 | 53,88 | 152,31 |
| 313,15 | 49,64 | 58,87 | 63,92 | 66,06 | 26,98 | 93,32 | 71,00 | 49,04 | 141,34 |
| 333,15 | 49,14 | 60,72 | 65,78 | 65,09 | 27,90 | 95,94 | 70,50 | 50,66 | 145,06 |
| 353,15 | 48,22 | 62,56 | 67,62 | 64,70 | 28,82 | 98,52 | 70,00 | 52,28 | 148,72 |
| 373,15 | 46,49 | 67,97 | 73,00 | 62,13 | 31,55 | 106,04 | 69,60 | 57,08 | 159,30 |

## COMPARISON WITH EXPERIMENTAL DATA (tentative)

Symbols: Exp. $=$ experimental Num. $=$ numerical Analít. $=$ analytical (Dunn et al., 1993)

Composites with DKA X type fibers (transverse conductivity)

| $\mathrm{T}(\mathrm{K})$ | $55 \%$ |  |  |  | $65 \%$ |  |  | $75 \%$ |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Exp. | Num. | Analít. | Exp. | Num. | Analít. | Exp. | Num. | Analít. |  |
| 293,15 | 6,80 | 3,41 | 3,21 | 9,10 | 5,51 | 4,39 | 7,83 | 14,46 | 6,50 |  |
| 313,15 | 6,80 | 3,08 | 2,90 | 9,08 | 4,98 | 3,96 | 7,81 | 13,09 | 5,88 |  |
| 333,15 | 6,76 | 3,19 | 3,00 | 8,97 | 5,15 | 4,10 | 7,79 | 13,55 | 6,08 |  |
| 353,15 | 6,75 | 3,30 | 3,10 | 8,80 | 5,33 | 4,25 | 7,79 | 14,00 | 6,29 |  |
| 373,15 | 6,65 | 3,63 | 3,41 | 8,80 | 5,86 | 4,67 | 7,74 | 15,37 | 6,92 |  |

Disordered array of cylinders with interfacial thermal resistance and pores ( $c_{p}=0,5 \%$ ) (novelty!)

Test case 1: $a=250$ e $\mathrm{Bi}=10$
Test case 2: $a=250$ e $\mathrm{Bi}=10^{-6}$
Test case 3: $k_{11}=k_{22}=k_{33}=250, k_{12}=k_{13}=k_{23}=200 \mathrm{e} \mathrm{Bi}=10$
Test case 4: $k_{11}=k_{22}=k_{33}=250, k_{12}=k_{13}=k_{23}=200 \mathrm{e} \mathrm{Bi}=10^{-6}$

| Test case | Effective thermal conductivity $c=13 \%$ and $\rho_{f}=1,5$ |  |  |
| :---: | :---: | :---: | :---: |
|  | $\kappa_{11}^{e_{1} h}$ | $\kappa_{22}^{\varepsilon_{1} h}$ | $\kappa_{33}^{\varepsilon_{1} h}$ |
| 1 | 1,299 | 1,189 | 1,083 |
| 2 | 0,8649 | 0,8497 | 0,8336 |
| 3 | 1,282 | 1,180 | 1,080 |
| 4 | 0,8650 | 0,8497 | 0,8336 |

## DOABLE FUTURE WORKS (i)

- Implementation of more representative 3-D geometric models for the microstructures of composite materials
- Implementation of variable interfacial thermal resistance on the surface of the fibers (Duschlbauer et al., 2003; Fletcher, 2001)
- Appropriate treatment of microscale for analysis of configurations that are close to maximum packing
- Extension of developed methodology to determine effective mechanical properties of composite materials (for example, effective elastic modulus
- Consideration of the effect of properties varying with temperature

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## Homogenization of Temperature-Dependent Thermal Conductivity in Composite Materials

## 

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Of the various homogenization approaches, the asymptotic expansion homogenization (AEH) approach for
 complex microstructural shapes while relating continuum fields of different scales. The objective is to study the AEH approach for nonlinear thermai heat conduction with e series. Under conditions of symmetry such as in unidirectional conposites, the two approache give the fraction and temperature. The validations are performed using measurements and analytical formulas available in the literature. The findings show good agreement between the present numerical predictions and independences Finally, a simple nonlinear steady-state heat conduction problem is demonstrated to illustrate the multi-scale procedure. The numerically predicted results are verified using a Runge-Kutta solution. are proposed to investigate the sensitivity of the homogenized conductivity to higher-order terms of the asymptotic

The smaller the magnitude of $\varepsilon$, the smaller the influence of the macrolevel temperature gradients on the microscale homogenized properties. Under certain conditions, the difference between the approaches is nominal. Conditions when the linearized and nonlinear homogenization equations yield identical or nearly identical results are 1) the microstructuralgeometry contains symmetries, 2) the ma-
terial is homogeneous, 3) $\partial T^{(0)} / \partial x=0$, and 4) $\varepsilon \ll 1$.

In summary, the steps in the proposed linear and nonlinear computational procedures are enumerated as follows.

The linear approach assumes that the temperatures are constant in $Y$. The procedure for determining the homogenized conductivity in a finite element sense is as follows:

1) Compute the macrotemperature distribution.
2) Determine the element average (at centroid or integration points) temperatures for each macrolevel element.
3) Determine the individual phase conductivities at the average temperature at each microlevel element.
4) Solve the auxiliaryequation(10) for $x^{j}$ using the conductivities from step 3 .
5) Use the
6) Use the solution for $\chi^{j}$ in Eq. (15) to determine the effective
conductivity of the macroelement.

## Nonlinear

The nonlinear approach make, no restrictions on the temperature distribution in $Y$. This results in a nonlinear dependence of
the homogenized conductivity on the local temperature fields. The procedure to determine the effective conductivity is as follows: 1) Compute the macrotemperature distribution.
2) Determine the element average (or centroid or integration points) temperatures for each macrolevel element. 3) Solve for $\chi^{\prime}$ in Eq. (12) using the conductivity values for the
present iteration. 4) Determine 4) Determine the microscale temperatures using the first two
terims in Eq. (4).
5) Update the conductivities of the constituents using the mi-
croscale temperatures.
6) Loop back to step 1 until $\chi^{j}$ converges.
5) Update the conductivities of the constituents using the mi-
croscale temperatures.
6) Loop back to step 1 until $\chi^{j}$ converges. corrector functions $\chi^{\prime}$.
Although limited developments

$$
\begin{aligned}
& \text { are available in homogenization oi linear conductivity, } 9.10 \text { no ef- } \\
& \text { forts to date have treated the nonlinear temperature dependence of } \\
& \text { conductivityor shownhow such approaches substantiatethe results. }
\end{aligned}
$$

## ACKNOWLEDGEMENTS

- PEM/COPPE/UFRJ
- CNPq
- FAPERJ
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- Current and former graduate and undergraduate students (room for more...)


## THE END !!

## THANK YOU !!

## ALGUNS TRABALHOS PUBLICADOS ATÉ O MOMENTO

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## Cálculo das contribuições associadas ao nó mediano $M$ em $\Gamma$

$>$ Definição da função peso $\left.\quad v_{M}\right|_{e, \Gamma}=\left.\phi_{M}^{c}\right|_{e, \Gamma}$
> Cálculo do salto da função peso

$$
\left[v_{M}\right]_{\Gamma_{e e^{\prime}}}=\left.v_{M}\right|_{e, \Gamma}-\overbrace{\left.v_{M}\right|_{e^{\prime}, \Gamma}}=\left.\phi_{M}^{c}\right|_{e, \Gamma}
$$

> Cálculo do salto da função teste

$$
\left[\chi_{p, h}^{\mathrm{II}}\right]_{\Gamma_{e e^{\prime}}}=\left.\chi_{p, h}^{\mathrm{II}, c}\right|_{e, \Gamma}-\chi_{p, h}^{\mathrm{II}, d} e_{e, \Gamma}
$$

$$
\text { somar ao componente } K_{M A}
$$

$$
\int_{\Gamma_{e e^{\prime}}} \operatorname{Bi}\left[v_{M}\right]_{\Gamma_{e e^{\prime}}}\left[\chi_{p, h}^{I I}\right]_{\Gamma_{e e^{\prime}}} d \mathbf{s}=\operatorname{Bi}\left(\left.\left.\chi_{A} \int_{\Gamma_{e e^{\prime}}} \phi_{M, \Gamma}^{c}\right|_{, \Gamma} \phi_{A}^{c}\right|_{e, \Gamma} d \mathbf{s}+\left.\left.\chi_{B} \int_{\Gamma_{e e^{\prime}}} \phi_{M, \Gamma}^{c}\right|_{e, \Gamma} ^{c} \phi_{B}^{c}\right|_{e, \Gamma} d \mathbf{s}+\right.
$$

$$
\left.\left.\chi_{C} \int_{\Gamma_{e e^{\prime}}} \phi_{M, \Gamma}^{c}\right|_{e, \Gamma} ^{c}\right|_{C, \Gamma} d \mathbf{s}+\left.\left.\chi_{M} \int_{\Gamma_{e e^{\prime}}} \phi_{M}^{c}\right|_{e, \Gamma} \phi_{M}^{c}\right|_{e, \Gamma} d \mathbf{s}+\left.\left.\chi_{N} \int_{\Gamma_{e e^{\prime}}} \phi_{M, \Gamma}^{c}\right|_{e, \Gamma} \phi_{N}^{c}\right|_{e, \Gamma} d \mathbf{s}+
$$

$$
\left.\left.\chi_{P} \int_{\Gamma_{e e^{\prime}}} \phi_{M, \Gamma}^{c}\right|_{e, \Gamma} \phi_{P}^{c}\right|_{e, \Gamma} d \mathbf{s}-\left.\left.\chi_{A^{\prime}} \int_{\Gamma_{r e^{\prime}}} \phi_{M, \Gamma}^{c}\right|_{e, \Gamma} \phi_{A^{\prime}}^{d}\left|e^{\prime}, \Gamma d \mathbf{s}-\chi_{\mathcal{B}^{\prime}} \int_{\Gamma_{e e^{\prime}}} \phi_{M, \Gamma}^{c}\right|_{e, \Gamma} \phi_{B^{\prime}}^{d}\right|_{e^{\prime}, \Gamma} d \mathbf{s}-
$$

$$
\chi_{C^{\prime}} \int_{\Gamma_{e e^{\prime}}} \phi_{M}^{c}\left|e, \Gamma \phi_{C^{\prime}}^{d}\right| e^{\prime}, \Gamma \mathrm{\Gamma} ~ d \mathbf{s}-\chi_{M^{\prime}} \int_{\Gamma_{e e^{\prime}}} \phi_{M}^{c}\left|e, \Gamma \phi_{M^{\prime}}^{d}\right| e^{\prime}, \Gamma d \mathbf{s}-\chi_{N^{\prime}} \int_{\Gamma_{e e^{\prime}}} \phi_{M}^{c}\left|e, \Gamma \phi_{N^{\prime}}^{d}\right| e^{\prime}, \Gamma d \mathbf{s}-
$$

$$
\left.\left.\chi_{P^{\prime}} \int_{\Gamma_{e e^{\prime}}} \phi_{M}^{c}\right|_{e, \Gamma} \phi_{P^{\prime}}^{d} \mid e_{e^{\prime}, \Gamma} d \mathbf{s}\right)
$$

$$
\begin{aligned}
& {\left[\chi_{p, h}^{\mathrm{II}}\right]_{\Gamma_{e e^{\prime}}}=\left.\chi_{A} \phi_{A}^{c}\right|_{e, \Gamma}+\left.\chi_{B} \phi_{B}^{c}\right|_{e, \Gamma}+\left.\chi_{C} \phi_{C}^{c}\right|_{e, \Gamma}+\chi_{M} \phi_{M}^{c}\left|e, \Gamma+\chi_{N} \phi_{N}^{c}\right|_{e, \Gamma}+\left.\chi_{P} \phi_{P}^{c}\right|_{e, \Gamma}-} \\
& \left.\chi_{A^{\prime}} \phi_{A^{\prime}}^{d}\right|_{e^{\prime}, \Gamma}-\left.\chi_{B^{\prime}} \phi_{B^{\prime}}^{d}\right|_{e, \Gamma}-\left.\chi_{C^{\prime}} \phi_{C^{\prime}}^{d}\right|_{e^{\prime}, \Gamma}-\left.\chi_{M^{\prime}} \phi_{M^{\prime}}^{d}\right|_{e^{e}, \Gamma}-\chi_{N^{\prime}} \phi_{N^{\prime}}^{d}\left|e^{\prime}, \Gamma-\chi_{P^{\prime}} \phi_{P^{\prime}}^{d}\right|_{e, \Gamma}
\end{aligned}
$$

## CÁLCULO DAS INTEGRAIS DE SUPERFÍCIE RESULTANTES



## NUMERICAL METHODS (vii)

- Finite element discretization
$>$ Cell problem

$$
\begin{gathered}
a\left(v, \chi_{p}^{\mathrm{II}}\right)+b_{\Gamma}\left(v, \chi_{p}^{\mathrm{II}}\right)=\ell(v) \quad \forall v \in Y^{\mathrm{II}}\left(\Omega_{p c}\right) \\
a\left(v, \chi_{p}^{\mathrm{II}}\right)=\int_{\Omega_{p c}} \zeta_{i j}(\mathbf{y}) \frac{\partial \chi_{p}^{\mathrm{II}}}{\partial y_{j}} \frac{\partial v}{\partial y_{i}} d \mathbf{y} \quad \begin{array}{l}
\text { bilinear operator, symmetric and } \\
\text { positive-definite }
\end{array} \\
\ell(v)=\int_{\Omega_{p c}} \zeta_{i p}(\mathrm{y}) \frac{\partial v}{\partial y_{i}} d \mathbf{y} \quad \begin{array}{l}
\text { linear functional related to direction of } \\
\text { temperature gradient imposed externally }
\end{array} \\
b_{\Gamma}\left(v, \chi_{p}^{\mathrm{II}}\right)=\int_{\Gamma} \mathrm{Bi}\left[\chi_{p}^{\mathrm{II}}\right]_{\Gamma}\left[v v_{\Gamma} d \mathrm{~s} \quad\right. \text { bilinear and symmetric operator }
\end{gathered}
$$

## NUMERICAL METHODS (viii)

- Finite element discretization


## > Treatment of volume integrals

Galerkin Method (Reddy, 1993; Hughes, 1987)

$$
\begin{aligned}
& \chi_{p}^{e} \equiv \chi_{p}^{\mathrm{II}} \mid \Omega_{\varepsilon}^{e}=\sum_{a=1}^{10} \chi_{p, \alpha}^{e} \psi_{a}^{e} \\
& v^{e} \equiv v \left\lvert\, \Omega^{e}=\sum_{b=1}^{10} v_{b}^{\epsilon} \psi_{b}^{e} \quad \ell\left(v^{e}\right) \rightarrow f_{a}^{e} \quad \mathbf{J}^{e}=\frac{\partial\left(y_{1}, y_{2}, y_{3}\right)}{\partial(\xi, \eta, \zeta)}\right. \\
& f_{a}^{e}=\int_{\Omega^{e}} \zeta_{i p}^{e} \frac{\partial \psi_{a}^{e}}{\partial y_{i}} d \mathbf{y}=\int_{0}^{1} \int_{0}^{1-\xi} \int_{0}^{1-\xi-\eta} \zeta_{i p}^{e}\left(\frac{\partial \psi_{a}^{e}}{\partial \xi} \frac{\partial \xi}{\partial y_{i}}+\frac{\partial \psi_{a}^{e}}{\partial \eta} \frac{\partial \eta}{\partial y_{i}}+\frac{\partial \psi_{a}^{e}}{\partial \zeta} \frac{\partial \zeta}{\partial y_{i}}\right) \operatorname{det} \mathbf{J}^{e} d \zeta d \eta d \xi \\
& k_{a b}^{e}=\int_{\Omega^{c}} \zeta_{i j}^{e} \frac{\partial \psi_{a}^{e}}{\partial y_{j}} \frac{\partial \psi_{a}^{e}}{\partial y_{i}} d y \\
& =\int_{0}^{1} \int_{0}^{1-\xi} \int_{0}^{1-\xi-\eta} \zeta_{i j}^{e}\left(\frac{\partial \psi_{a}^{e}}{\partial \xi} \frac{\partial \xi}{\partial y_{j}}+\frac{\partial \psi_{a}^{e}}{\partial \eta} \frac{\partial \eta}{\partial y_{j}}+\frac{\partial \psi_{a}^{e}}{\partial \zeta} \frac{\partial \zeta}{\partial y_{j}}\right)\left(\frac{\partial \psi_{b}^{e}}{\partial \xi} \frac{\partial \xi}{\partial y_{j}}+\frac{\partial \psi_{b}^{e}}{\partial \eta} \frac{\partial \eta}{\partial y_{j}}+\frac{\partial \psi_{b}^{e}}{\partial \zeta} \frac{\partial \zeta}{\partial y_{j}}\right) \operatorname{det} \mathbf{J}^{e} d \zeta d \eta d \xi
\end{aligned}
$$

## NUMERICAL METHODS (ix)

- Finite element discretization
> Treatment of surface integral
$\checkmark$ Duplication of degrees of freedom associated with global nodes situated on the interface Gamma.
$\checkmark$ Modification of connectivity of tetrahedra that possess at least one node on Gamma.
$\checkmark$ Calculation of the jumps of the functions in the integrand through the element surfaces on Gamma.
$\checkmark$ Integration of the products of the jumps over Gamma.
$\checkmark$ Sum of the resulting integrals to the appropriate components in the global stiffness matrix.


## Duplication of degrees of freedom.

Modification of connectivity of tetrahedra.

## BEFORE DUPLICATION



AFTER DUPLICATION


## NUMERICAL METHODS (x)

- Contributions associated with node of vertex $A$
$>$ Weight function restricted to node $A$

$$
\left.v_{A}\right|_{e, \Gamma}=\left.\phi_{A}^{c}\right|_{e, \Gamma}
$$

$>$ Jump of weight function across Gamma $_{\mathrm{ee}}$,

$$
\left[v_{A}\right]_{\Gamma e e^{\prime}}=\left.v_{A}\right|_{e, \Gamma}-\overbrace{\left.v_{A}\right|_{e, \Gamma}}^{0}=\left.v_{A}\right|_{e, \Gamma}=\left.\phi_{A}^{c}\right|_{e, \Gamma}
$$

$>$ Jump of temperature across Gamma ${ }_{\text {ee }}\left[\chi_{p, h}^{\mathrm{I}}\right]_{\Gamma_{e^{\prime}}}=\left.\chi_{p, h, h, \Gamma}^{\mathrm{II} c}\right|_{e, \Gamma}-\chi_{p, h}^{\mathrm{II}, d} e_{e, \Gamma}$

$$
\begin{aligned}
& {\left[\chi_{p, h}^{I I}\right]_{\Gamma_{e e^{\prime}}}=\left.\chi_{A} \phi_{A}^{c}\right|_{e, \Gamma}+\left.\chi_{B} \phi_{B}^{c}\right|_{e, \Gamma}+\left.\chi_{C} \phi_{C}^{c}\right|_{e, \Gamma}+\left.\chi_{M} \phi_{M}^{c}\right|_{e, \Gamma}+\left.\chi_{N} \phi_{N}^{c}\right|_{e, \Gamma}+\left.\chi_{P} \phi_{P}^{c}\right|_{e, \Gamma}-} \\
& \left.\chi_{A^{\prime}} \phi_{A^{\prime}}^{d}\right|_{e^{\prime}, \Gamma}-\left.\chi_{B^{\prime}} \phi_{B^{\prime}}^{d}\right|_{e^{\prime}, \Gamma}-\left.\chi_{C^{\prime}} \phi_{C^{\prime}}^{d}\right|_{e^{\prime}, \Gamma}-\left.\chi_{M^{\prime}} \phi_{M^{\prime}}^{d}\right|_{e^{\prime}, \Gamma}-\left.\chi_{N^{\prime}} \phi_{N^{\prime}}^{d}\right|_{e^{\prime}, \Gamma}-\left.\chi_{P^{\prime}} \phi_{P^{\prime}}^{d}\right|_{e^{\prime}, \Gamma}
\end{aligned}
$$

## NUMERICAL METHODS (xi)

- Contributions associated with node of vertex $A$

$$
\begin{array}{r}
\text { sum to component } K_{A A} \\
\int_{\Gamma_{e e^{\prime}}} \operatorname{Bi}\left[v_{A}\right]_{\Gamma_{e e^{\prime}}}\left[\chi_{p, h}^{I I}\right]_{\Gamma_{e e^{\prime}}} d \mathbf{s}=\operatorname{Bi}\left(\left.\chi_{A}\left|\int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{A}^{c}\right|_{e, \Gamma} d \mathbf{s}\right)+\left.\left.\chi_{B} \int_{\Gamma_{e e^{\prime}}} \phi_{A, \Gamma}^{c}\right|_{e, \Gamma} \phi_{B}^{c}\right|_{e, \Gamma} d \mathbf{s}+ \\
\left.\left.\chi_{C} \int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{C}^{c}\right|_{e, \Gamma} d \mathbf{s}+\left.\left.\chi_{M} \int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{M}^{c}\right|_{e, \Gamma} d \mathbf{s}+\left.\left.\chi_{N} \int_{\Gamma_{e e^{\prime}}} \phi_{A, \Gamma}^{c}\right|_{e, \Gamma} \phi_{N}^{c}\right|_{e, \Gamma} d \mathbf{s}+ \\
\left.\left.\chi_{P} \int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{P}^{c}\right|_{e, \Gamma} d \mathbf{s}-\left.\left.\chi_{A^{\prime}} \int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{A^{\prime}}^{d}\right|_{e^{\prime}, \Gamma} d \mathbf{s}-\left.\left.\chi_{B^{\prime}} \int_{\Gamma_{e e^{\prime}}} \phi_{A, \Gamma}^{c}\right|_{e, \Gamma} \phi_{B^{\prime}}^{d}\right|_{e^{\prime}, \Gamma} d \mathbf{s}- \\
\left.\left.\chi_{C^{\prime}} \int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{C^{\prime}}^{d}\right|_{e^{\prime}, \Gamma} d \mathbf{s}-\left.\left.\chi_{M^{\prime}} \int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{M^{\prime}}^{d}\right|_{e^{\prime}, \Gamma} d \mathbf{s}-\left.\left.\chi_{N^{\prime}} \int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{N^{\prime}}^{d}\right|_{e^{\prime}, \Gamma} d \mathbf{s}- \\
\left.\left.\left.\chi_{P^{\prime}} \int_{\Gamma_{e e^{\prime}}} \phi_{A}^{c}\right|_{e, \Gamma} \phi_{P^{\prime}}^{d}\right|_{e^{\prime}, \Gamma} d \mathbf{s}\right)
\end{array}
$$

## NUMERICAL METHODS (xii)

- Algorithm

For each node situated on Gamma
$>$ Identification of neighboring nodes (corner and median).
$>$ Identification of its duplicates and of duplicates of neighboring nodes.
$>$ Definition of weight function restricted to node and to tetrahedra which share the node on Gamma.
$>$ Calculation of jumps of weight and temperature functions across tetrahedra surfaces which share the node on Gamma.
$>$ Evaluation of resulting integrals.
$>$ Sum of resulting integrals to the appropriate components in the global stiffness matrix.

## NUMERICAL METHODS (xiii)

- Discrete system of equations

$$
\mathcal{K}^{*} \boldsymbol{\chi}_{p, h}^{\mathrm{II}}=\mathcal{F}^{*}
$$

Global stiffness matrix and global forcing vector are assembled from elemental matrices and elemental vectors, imposing periodic boundary conditions on the outer surfaces of Omega ${ }_{p c}$.

## NUMERICAL METHODS (xiv)

- Iterative method

Global minimum residual, GMRES (Paige \& Saunders, 1975)
> Appropriate for linear systems of equations whose coefficient matrices are symmetric, but not necessarily positive-definite.
$>$ Stopping criterion: based on the norm $L_{2}$ of the residual vector, subject to a user-prescribed tolerance Sigma.

$$
\mathbf{A} \mathbf{u}=\mathbf{b}
$$

$$
\begin{aligned}
& \mathbf{r} \equiv \mathbf{b}-\mathbf{A} \mathbf{u}^{*} \mathbf{r}_{0} \equiv \mathbf{b}-\mathbf{A} \mathbf{u}^{*(0)} \\
&\|\mathbf{r}\|_{L_{2}}=\left(\mathbf{r}^{T} \mathbf{r}\right)^{1 / 2}\left\|\mathbf{r}_{0}\right\|_{L_{2}}=\left(\mathbf{r}_{0}^{T} \mathbf{r}_{0}\right) \\
& \frac{\|\mathbf{r}\|_{L_{2}}}{\left\|\mathbf{r}_{0}\right\|_{L_{2}}}<\sigma^{2}
\end{aligned}
$$

## RESULTS

- 2-D effort: 'smaller' than the 3-D effort, and it is (still) valuable for random arrangements.
- Simple cubic array of spheres with uniform interfacial thermal resistance (and, also, with perfect thermal contact).
- Disordered array of spheres with uniform interfacial thermal resistance and pores in the matrix (illustrative computations).
- Parallelepipedonal array of cylinders with uniform interfacial thermal resistance.
- Comparison with experimental data: still tentative!

DETERMINAÇÃO DA CONDUTIVIDADE TÉRMICA EFETIVA DE COMPÓSITOS FIBROSOS UNIDIRECIONAIS RANDÔMICOS

Leandro Bastos Machado

Figura 6.8: A célula de Voronoi com 17 fibras e $c=0,375$.


## Tool developed, but not systematically used.



Figura 6.10: Malha para as realizações com 32 fibras e $c=0,5$.

#  

## BOUNDS FOR THE EFFECTIVE CONDUCTIVITY OF UNIDIRECTIONAL COMPOSITES BASED ON ISOTROPIC MICROSCALE MODELS

## Leandro B. Machado

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Microscale models validated.
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(a)

(b)

Figura 6.1: Células periódicas dos arranjos ordenados triangular (a) e quadrado (b).


Figure 2: Illustrative finite element meshes for the square array, $c=0.75$ : mesh on the left is for $\Omega_{p c}(\mathcal{N}=0)$, and mesh on the right is for both $\mathcal{L}$ and $\mathcal{U}(\mathcal{N}=2)$.

| $c$ | $\alpha$ |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 2 |  |  | 10 |  |  | 50 |  |  |
| 0.75 | $\beta$ | $k_{e}$ | $k_{e, h}$ | $\beta$ | $k_{\text {e }}$ | $k_{\text {e, }}$ | $\beta$ | $k_{e}$ | $k_{e, h}$ |
|  |  | 1.6767 | 1.677 |  | 4.9443 | 4.946 |  | 9.5355 | 9.546 |
|  | 0.06 | $k_{\text {LB,h }}$ | $k_{\text {UB, } h}$ | 0.06 | $k_{\text {LB,h }}$ | $k_{\text {UB }, h}$ | 0.06 | $k_{\text {LB,h }}$ | $k_{\text {UB, } h}$ |
|  |  | 1.620 | 1.686 |  | 4.240 | 5.833 |  | 6.793 | 23.61 |
|  |  | $\bar{k}_{e, h}$ | $\bar{E}_{r}$ |  | $\bar{k}_{e, h}$ | $\bar{E}_{r}$ |  | $\bar{k}_{e, h}$ | $\overline{\bar{E}}_{r}$ |
|  |  | 1.65 | 2.0\% |  | 5.0 | 16\% |  | 15 | 56\% |
|  | 0.04 | $k_{\mathrm{LB}, \mathrm{h}}$ | $k_{\text {UB,h }}$ | 0.04 | $k_{\text {LB,h }}$ | $k_{\text {UB }, \mathrm{h}}$ | 0.04 | $k_{\text {LB,h }}$ | $k_{\text {UB, }, ~}$ |
|  |  | 1.647 | 1.683 |  | 4.524 | 5.653 |  | 7.714 | 21.77 |
|  |  | $\bar{k}_{e, h}$ | $\bar{E}_{r}$ |  | $\bar{k}_{e, h}$ | $\bar{E}_{5}$ |  | $\bar{k}_{e, h}$ | $\bar{E}_{r}$ |
|  |  | 1.67 | 1.1\% |  | 5.1 | 11\% |  | 15 | 47\% |
| 0.78 | $\beta$ | $k_{e}$ | $k_{e, h}$ | $\beta$ | $k_{\text {e }}$ | $k_{\text {c, } h}$ | $\beta$ | $k_{\text {c }}$ | $k_{\text {e, } h}$ |
|  |  | 1.7154 | 1.715 |  | 5.8037 | 5.805 |  | 16.310 | 16.32 |
|  | 0.06 | $k_{\text {LB, } h}$ | KUB,h | 0.06 | $k_{\text {LB, } h}$ | $k_{\text {UB, } h}$ | 0.06 | $k_{\text {LB,h }}$ | $k_{U B, h}$ |
|  |  | 1.671 | 1.719 |  | 4.983 | 6.126 |  | 9.575 | 24.66 |
|  |  | $\bar{k}_{\text {e,h }}$ | $\bar{E}_{r}$ |  | $\bar{k}_{e, h}$ | $\bar{E}_{r}$ |  | $\bar{k}_{e, h}$ | $\bar{E}_{r}$ |
|  |  | 1.70 | 1.4\% |  | 5.6 | 10\% |  | 17 | 44\% |
|  | 0.04 | $k_{\text {LB,h }}$ | $k_{\text {UB, } h}$ | 0.04 | $k_{\text {LB,h }}$ | $k_{\text {UB, } h}$ | 0.04 | $k_{\text {LB, } h}$ | $k_{\text {UB, } h}$ |
|  |  | 1.695 | 1.717 |  | 5.369 | 6.004 |  | 11.76 | 22.96 |
|  |  | $\bar{k}_{e, h}$ | $\bar{E}_{\text {E }}$ |  | $\bar{k}_{e, h}$ | $\bar{E}_{r}$ |  | $\bar{k}_{e, h}$ | $\bar{E}_{r}$ |
|  |  | 1.71 | 0.64\% |  | 5.7 | 5.6\% |  | 17 | 33\% |
| 0.785 | $\hat{\beta}$ | $k_{e}$ | $k_{\text {e, } h}$ | $\beta$ | $k_{\text {e }}$ | $k_{e, h}$ | $\beta$ | $k_{\text {e }}$ | $k_{e, h}$ |
|  |  | 1.7220 | - |  | 6.004 | - |  | 20.5 | - |
|  | 0.06 | $k_{\text {LB,h }}$ | $k_{\text {UB,h }}$ | 0.06 | $k_{\text {LB,h }}$ | $k_{\text {UB,h }}$ | 0.06 | $k_{\text {LB,h }}$ | $k_{\text {UB, } h}$ |
|  |  | 1.680 | 1.724 |  | 5.16 | 6.19 |  | 10.5 | 24.9 |
|  |  | $\bar{k}_{e, h}$ | $\bar{E}_{r}$ |  | $\bar{k}_{e, h}$ | $\bar{E}_{r}$ |  | $\bar{k}_{e, h}$ | $\bar{E}_{r}$ |
|  |  | 1.70 | 1.3\% |  | 5.7 | 9.0\% |  | 18 | 41\% |
|  | 0.04 | $\bar{k}_{\text {LB,h }}$ | KUB,h | 0.04 | $k_{\text {LB,h }}$ | $k_{U B, h}$ | 0.04 | $k_{\text {LB,h }}$ | kUB, $h$ |
|  |  | 1.704 | 1.723 |  | 5.59 | 6.08 |  | 13.5 | 23.3 |
|  |  | $\bar{k}_{e, h}$ | $\bar{E}_{r}$ |  | $\bar{k}_{e, h}$ | $\bar{E}_{r}$ |  | $\bar{k}_{e, h}$ | $\bar{E}_{r}$ |
|  |  | 1.713 | 0.55\% |  | 5.8 | 4.2\% |  | 18 | 27\% |
| $\pi / 4$ | $\beta$ | $k_{e}$ | $k_{e, h}$ | $\beta$ | $k_{\text {c }}$ | $k_{e, h}$ | $\beta$ | $k_{e}$ | $k_{e, h}$ |
|  |  | - | - |  | - | - |  | - | - |
|  | 0.06 | $k_{\text {LB,h }}$ | $k_{\text {UB, } h}$ | 0.06 | $k_{\text {LB, } h}$ | $k_{\cup B, h}$ | 0.06 | $k_{\text {LB,h }}$ | KUB, h |
|  |  | 1.681 | 1.725 |  | 5.18 | 6.19 |  | 10.6 | 24.9 |
|  |  | $\bar{k}_{e, h}$ | $\bar{E}_{r}$ |  | $\bar{k}_{e, h}$ | $\bar{E}_{r}$ |  | $\bar{k}_{e, h}$ | $\bar{E}_{r}$ |
|  |  | 1.70 | 1.3\% |  | 5.7 | 8.9\% |  | 18 | 40\% |
|  | 0.04 | $k_{L B, h}$ | kUB, $h$ | 0.04 | $k_{\text {LB, } h}$ | $k_{\text {UB, } h}$ | 0.04 | $k_{L B, h}$ | KUB, $h$ |
|  |  | 1.705 | 1.723 |  | 5.61 | 6.09 |  | 13.7 | 23.3 |
|  |  | $\bar{k}_{e, h}$ | $\bar{E}_{\text {r }}$ |  | $\bar{k}_{e, h}$ | $\bar{E}_{r}$ |  | $\bar{k}_{e, h}$ | $E_{r}$ |
|  |  | 1.714 | 0.53\% |  | 5.9 | 4.1\% |  | 18 | 26\% |

Table 1: Effective conductivity results for the square array Parameters: $c \in\{0.75,0.78,0.785, \pi / 4\}, \alpha \in\{2,10,50\}$,

$$
\beta \in\{0.04,0.06\} .
$$



Figura 6.14: Célula de Voronoi com 32 fibras e $c=0,5$, onde a malha só pode ser gerada com a eliminação de regiões de estreito.

Tabela 6.10: Resultados obtidos para as realizações com 32 fibras, $c=0,5$ e $\alpha \in$ $\{2,10,50\}$, onde a geração de malha é possível: numéricos, $k_{e, h}$, limites isotrópicos, $k_{\mathrm{II}, h}$ e $k_{\mathrm{SI}, h}$, limitєS anisotrópicos, $k_{\mathrm{IA}, h}$ e $k_{\mathrm{SA}, h}$, estimativas para a condutividade, $\bar{k}_{\mathrm{I}}$ e $\vec{k}_{\mathrm{A}}$, e erros relativos, $\bar{E}_{r, I}$ e $\bar{E}_{r, \mathrm{~A}}$. Parâmetros das regiões de estreito: $\beta=0,06 \mathrm{e}$ $\gamma_{c}=0,1$. Microscale models useful.

| $\alpha=2$ |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $k_{e, h}$ | $k_{11, h}$ | $k_{\text {Sl,h }}$ | $\bar{k}_{1}$ | $\bar{E}_{r, 1}$ | $k_{1 \mathrm{~A}, h}$ | $k_{\text {SA, } h}$ | $\bar{k}_{\text {A }}$ | $\bar{E}_{r, A}$ |
| 1,410 | 1,397 | 1,413 | 1,4 | 5,5\% | 1,398 | 1,412 | 1,4 | 5,2\% |
| $\alpha=10$ |  |  |  |  |  |  |  |  |
| $k_{e, h}$ | $k_{11, h}$ | $k_{\text {Sl,h }}$ | $\bar{k}_{1}$ | $\bar{E}_{r, 1}$ | $k_{\text {IA, }, ~}$ | $k_{\text {SA }, h}$ | $\bar{k}_{\text {A }}$ | $\bar{E}_{r, A}$ |
| 2,636 | 2,545 | 2,768 | 2,7 | 4,2\% | 2,545 | 2,758 | 2,7 | 4,0\% |
| $\alpha=50$ |  |  |  |  |  |  |  |  |
| $k_{e, h}$ | $k_{11, h}$ | $k_{\text {Sl, } h}$ | $\bar{k}_{1}$ | $\bar{E}_{r, 1}$ | $k_{\text {IA,h }}$ | $k_{\text {SA, } h}$ | $\bar{k}_{\text {A }}$ | $\bar{E}_{r, A}$ |
| 3,454 | 3,239 | 4,134 | 3,7 | 12\% | 3,239 | 4,067 | 3,7 | 11\% |

## Extension

to 3-D
cubic
array

Microscale
models can be useful in 3-D.

## ABSTRACT SUBMISSION

Authors should submit two copies of an abstract of approximately 500 words. Authors and co-authors are requested to provide their complete addresses, phone and fax numbers, and e -mail addresses.

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## Simple cubic array of spheres

Validation with semi-analytical results by Cheng \& Torquato (1997)

$$
R_{c}=\kappa-1
$$

critical thermal contact resistance

| $c$ | $\alpha=10, R_{c}=9$ |  |  |  | $\alpha=10000, R_{c}=9999$ |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $R=5$ |  | $R=30$ |  | $R=5000$ |  | $R=20000$ |  |
|  | $\kappa_{e}^{h}$ | $\kappa_{e}^{\mathrm{CT}}$ | $\kappa_{e}^{h}$ | $\kappa_{e}^{\mathrm{CT}}$ | $\kappa_{e}^{h}$ | $\kappa_{e}^{\mathrm{CT}}$ | $\kappa_{e}^{h}$ | $\kappa_{e}^{\mathrm{CT}}$ |
| 0,05 | 1,0275 | 1,0275 | 0,9569 | 0,9569 | 1,0379 | 1,0380 | 0,9703 | 0,9703 |
| 0,10 | 1,0556 | 1,0556 | 0,9150 | 0,9150 | 1,0768 | 1,0769 | 0,9412 | 0,9412 |
| 0,15 | 1,0841 | 1,0841 | 0,8742 | 0,8742 | 1,1168 | 1,1168 | 0,9126 | 0,9126 |
| 0,20 | 1,1131 | 1,1132 | 0,8348 | 0,8348 | 1,1577 | 1,1578 | 0,8845 | 0,8845 |
| 0,25 | 1,1428 | 1,1428 | 0,7957 | 0,7957 | 1,1997 | 1,1998 | 0,8569 | 0,8569 |
| 0,30 | 1,1728 | 1,1729 | 0,7577 | 0,7577 | 1,2428 | 1,2429 | 0,8299 | 0,8298 |
| 0,35 | 1,2036 | 1,2036 | 0,7203 | 0,7203 | 1,2870 | 1,2870 | 0,8030 | 0,8029 |
| 0,40 | 1,2346 | 1,2347 | 0,6834 | 0,6833 | 1,3321 | 1,3322 | 0,7764 | 0,7763 |
| 0,45 | 1,2663 | 1,2663 | 0,6465 | 0,6464 | 1,3783 | 1,3783 | 0,7499 | 0,7498 |
| 0,50 | 1,2983 | 1,2983 | 0,6092 | 0,6091 | 1,4255 | 1,4254 | 0,7234 | 0,7232 |
| 0,51 | 1,3047 | 1,3047 | 0,6016 | 0,6015 | 1,4349 | 1,4349 | 0,7180 | 0,7178 |

Simple cubic array of spheres with uniform interfacial thermal resistance
Validation with semi-analytical results by Cheng \& Torquato (1997)
Convergence plots of absolute error


## Simple cubic array of spheres

Distinct behaviors for the effective thermal conductivity as a function of the magnitude of the interfacial thermal resistance


Disordered array of spheres with uniform interfacial thermal resistance and pores within the matrix Illustrative calculations, accurate: novelty!

| Values of $k_{e}^{\mathrm{N}}(\mathcal{C})$ for $c=0.15$ |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
| $\alpha=10$ |  |  |  |  |
| $R_{c}=9$ |  |  |  |  |
| Without voids |  |  |  |  |
| $\mathcal{C}$ | $R=5$ | $R=30$ | $R=5$ | $R=30$ |
| 1 | 1.0286 | 0.8509 | 1.0256 | 0.8469 |
| 2 | 1.0284 | 0.8466 | 1.0250 | 0.8440 |
| 3 | 1.0288 | 0.8571 | 1.0254 | 0.8543 |
| 4 | 1.0286 | 0.8518 | 1.0253 | 0.8490 |
| 5 | 1.0287 | 0.8557 | 1.0257 | 0.8525 |
| 6 | 1.0287 | 0.8535 | 1.0255 | 0.8502 |
| 7 | 1.0284 | 0.8462 | 1.0252 | 0.8424 |
| 8 | 1.0287 | 0.8548 | 1.0256 | 0.8502 |
| 9 | 1.0282 | 0.8409 | 1.0251 | 0.8371 |
| 10 | 1.0280 | 0.8337 | 1.0248 | 0.8305 |
| $k_{e}^{\mathrm{N}}$ | 1.0285 | 0.849 | 1.0253 | 0.846 |
| $S_{k_{e}^{\mathrm{N}}}$ | 0.0003 | 0.007 | 0.0003 | 0.007 |
| $k_{e}^{\mathrm{B}}$ | 1.0308 | 0.851 | - | - |


| Values of $k_{e}^{\mathrm{N}}(\mathcal{C})$ for $c=0.15$ |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $\alpha=10000, R_{c}=9999$ |  |  |  |  |  |
| Without voids |  |  |  |  |  |
| $\mathcal{C}$ | $R=5000$ | $R=20000$ | $R=5000$ | $R=20000$ |  |
| 1 | 1.0497 | 0.8789 | 1.0469 | 0.8751 |  |
| 2 | 1.0492 | 0.8761 | 1.0457 | 0.8733 |  |
| 3 | 1.0505 | 0.8831 | 1.0470 | 0.8802 |  |
| 4 | 1.0498 | 0.8795 | 1.0465 | 0.8766 |  |
| 5 | 1.0503 | 0.8821 | 1.0472 | 0.8790 |  |
| 6 | 1.0500 | 0.8807 | 1.0469 | 0.8774 |  |
| 7 | 1.0492 | 0.8758 | 1.0460 | 0.8721 |  |
| 8 | 1.0502 | 0.8816 | 1.0473 | 0.8772 |  |
| 9 | 1.0487 | 0.8724 | 1.0457 | 0.8688 |  |
| 10 | 1.0480 | 0.8678 | 1.0448 | 0.8646 |  |
|  | With $0.56 \%$ voids |  |  |  |  |
| $k_{e}^{\mathrm{N}}$ | 1.0496 | 0.878 | 1.0464 | 0.874 |  |
| $S_{k_{\mathrm{e}}^{\mathrm{N}}}$ | 0.0008 | 0.005 | 0.0008 | 0.005 |  |
| $k_{e}^{\mathrm{B}}$ | 1.0522 | 0.880 | - | - |  |

## Parallelepipedonal array of cylinders (Matt \& Cruz, 2006)

Validation against rule-of-mixtures results, and results from the expression by Hasselman \& Johnson (1987) for unidirectional fibrous composites with low $c$.

| $c=0,10, \rho_{p}=5 \mathrm{e} \alpha=100$ |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\rho_{f}$ | $\mathrm{Bi}=10^{-6}$ |  | $\mathrm{Bi}=10^{-1}$ |  | $\mathrm{Bi}=10^{2}$ |  |
|  | $\kappa_{11}^{e, h}$ | $\kappa_{22}^{e, h}$ | $\kappa_{11}^{e, h}$ | $\kappa_{22}^{e, h}$ | $\kappa_{11}^{e, h}$ | $\kappa_{22}^{e, h}$ |
| 6 | 0,8852 | 0,8335 | 0,9619 | 0,8401 | 1,9352 | 1,2283 |
| 8 | 0,8902 | 0,8286 | 0,9991 | 0,8349 | 2,3972 | 1,2160 |
| 12 | 0,8956 | 0,8226 | 1,0839 | 0,8285 | 4,1371 | 1,2023 |
| 13,5 | 0,8981 | 0,8204 | 1,1214 | 0,8262 | 5,8827 | 1,1964 |
| $\rho_{t, \max }=14$ | 10,900 | 0,8182 | 10,900 | 0,8240 | 10,900 | 1,1920 |
|  | $\kappa_{e, \mathrm{~L}}^{\mathrm{RM}}$ | $\kappa_{e, T}^{\mathrm{H}}$ | $\kappa_{e, \mathrm{~L}}^{\mathrm{RM}}$ | $\kappa_{e, T}^{\mathrm{H}}$ | $\kappa_{e, \mathrm{~L}}^{\mathrm{RM}}$ | $\kappa_{e, T}^{\mathrm{H}}$ |
|  | 10,900 | 0,8182 | 10,900 | 0,8240 | 10,900 | 1,1920 |

## Parallelepipedonal array of cylinders

Sample of new results!

Parallelepipedonal array $\rho_{p}=\rho_{f}=20$

| c | $\alpha=10$ |  |  |  | $\alpha=1000$ |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $\mathrm{Bi}=10^{-6}$ |  | $\mathrm{Bi}=10^{4}$ |  | $\mathrm{Bi}=10^{-6}$ |  | $\mathrm{Bi}=10^{4}$ |  |
|  | $\kappa_{11}^{e, h}$ | $\kappa_{22}^{e, h}$ | $\kappa_{11}^{e, h}$ | $\kappa_{22}^{e, h}$ | $\kappa_{11}^{e, h}$ | $\kappa_{22}^{e, h}$ | $\kappa_{11}^{e, h}$ | $\kappa_{22}^{e, h}$ |
| 0,10 | 0,8872 | 0,8356 | 1,4647 | 1,2005 | 0,8872 | 0,8356 | 1,9586 | 1,2586 |
| 0,20 | 0,7710 | 0,6971 | 1,8674 | 1,4490 | 0,7710 | 0,6971 | 2,6674 | 1,5990 |
| 0,30 | 0,6584 | 0,5743 | 2,3184 | 1,7568 | 0,6584 | 0,5743 | 3,5628 | 2,0540 |
| 0,40 | 0,5520 | 0,4613 | 2,8671 | 2,1432 | 0,5520 | 0,4613 | 4,8528 | 2,6847 |
| 0,50 | 0,4530 | 0,3541 | 3,5772 | 2,6441 | 0,453 | 0,354 | 6,977 | 3,627 |
| 0,60 | 0,3619 | 0,2492 | 4,5568 | 3,3292 | 0,362 | 0,249 | 11,27 | 5,244 |
| 0,70 | 0,2785 | 0,1406 | 6,0220 | 4,3667 | 0,278 | 0,141 | 25,03 | 9,094 |

Disordered array of cylinders with interfacial thermal resistance and pores ( $c_{\text {pores }}=0,5 \%$ ) (novelty!)

Test case 1: $a=250 \mathrm{e} \mathrm{Bi}=10$
Test case 2: $a=250 \mathrm{e} \mathrm{Bi}=10^{-6}$
Test case 3: $k_{11}=k_{22}=k_{33}=250, k_{12}=k_{13}=k_{23}=200 \mathrm{e} \mathrm{Bi}=10$
Test case 4: $k_{11}=k_{22}=k_{33}=250, k_{12}=k_{13}=k_{23}=200 \mathrm{e} \mathrm{Bi}=10^{-6}$

| Test case | Effective thermal conductivity $c=13 \%$ and $\rho_{f}=1,5$ |  |  |
| :---: | :---: | :---: | :---: |
|  | $\kappa_{11}^{e_{1} h}$ | $\kappa_{22}^{\varepsilon_{1} h}$ | $\kappa_{33}^{e_{1} h}$ |
| 1 | 1,299 | 1,189 | 1,083 |
| 2 | 0,8649 | 0,8497 | 0,8336 |
| 3 | 1,282 | 1,180 | 1,080 |
| 4 | 0,8650 | 0,8497 | 0,8336 |

## DOABLE FUTURE WORKS

- Implementation of more representative 3-D geometrical models for the microstructures of composite materials.
- Implementation of variable interfacial thermal resistance on the surface of the fibers (Duschlbauer et al., 2003; Fletcher, 2001).
- Appropriate treatment of microscale for analysis of configurations that are close to maximum packing.
- Extension of developed methodology to determine effective mechanical properties of composite materials (for example, effective elastic moduli).
- Consideration of the effect of properties varying with temperature.


## Temperature dependence.

# Homogenization of Temperature-Dependent Thermal Conductivity in Composite Materials 

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#### Abstract

Of the various homogenization approaches, the asymptotic expansion homogenization (AEH) approach for homogenizing nonlinear composite material properties continues to grow in prominence due to its ability to handle complex microstructural shapes while relating continuum fields of different scales. The objective is to study the AEH approach for nonlinear thermal heat conduction with temperature-dependent conductivity. First, two approaches are proposed to investigate the sensitivity of the homogenized conductivity to higher-order terms of the asymptotic series. Under conditions of symmetry such as in unidirectional composites, the two approaches give the same homogenized properties. Then validations are shown for unidirectional composites for changing volume fraction and temperature. The validations are performed using measurements and analytical formulas available in the literature. The findings show good agreemient between the present numerical predictions and independent results. Finally, a simple nonlinear steady-state heat conduction problem is demonstrated to illustrate the multi-scale procedure. The numerically predicted results are verified using a Runge-Kutta solution.


The sinaller the magnitude of $\varepsilon$, the smaller the influence of the macrolevel temperature gradients on the microscale homogenized properties. Under certain conditions, the difference between the approaches is nominal. Conditions when the linearized and nonlinear homogenization equations yield identical or nearly identical results are 1) the microstructural geometry contains symmetries, 2) the material is homogeneous, 3) $\partial T^{(0)} / \partial x=0$, and 4) $\varepsilon \lll 1$.

In summary, the steps in the proposed linear and nonlinear computational procedures are enumerated as follows.

## Linear

The linear approach assumes that the temperatures are constant in $Y$. The procedure for determining the homogenized conductivity in a finite element sense is as follows:

1) Compute the macrotemperature distribution.
2) Determine the element average (at centroid or integration points) temperatures for each macrolevel element.
3) Determine the individual phase conductivities at the average temperature at each microlevel element.
4) Solve the auxiliaryequation(10) for $\chi^{j}$ using the conductivities from step 3.
5) Use the solution for $\chi^{j}$ in Eq. (15) to determine the effective conductivity of the macroelement.

## Nonlinear

The nonlinear approach makes no restrictions on the temperature distribution in $Y$. This results in a nonlinear dependence of the homogenized conductivity on the local temperature fields. The procedure to determine the effective conductivity is as follows:

1) Compute the macrotemperature distribution.
2) Determine the element average (or centroid or integration points) temperatures for each macrolevel element.
3) Solve for $\chi^{j}$ in Eq. (12) using the conductivity values for the present iteration.
4) Determine the microscale temperatures using the first two terins in Eq. (4).
5) Update the conductivities of the constituents using the microscale temperatures.
6) I.oop back to step 1 until $\chi^{j}$ converges.
7) The effectiveconductivityis then computed from the converged corrector functions $\chi^{\prime}$.

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- FAPERJ
- CAPES
- Current and former graduate and undergraduate students (room for more...)


## THE END !!

## THANK YOU !!


[^0]:    7. D. A. G. bruggeman, Annal. Physik 24 (1935) 636.
