



# Computational approaches for heat conduction in composite materials

M.E. Cruz

*Department of Mechanical Engineering,  
EE/COPPE/Federal University of Rio de Janeiro, Brazil*

## Abstract

In this paper we consider computational approaches for the study of heat conduction in composite materials. Also, because of their importance to the validation of numerical results, we provide a brief overview of related analytical and experimental approaches. Sample analyses are presented, where representative numerical results for the effective thermal conductivity of fibrous and particulate composites are compared among themselves, and to some analytical predictions and experimental measurements. We conclude that still much work needs to be done in the field, in particular on the geometric and physical modeling of three-dimensional heat conduction in the composites in use today.

## 1 Introduction

Composite materials, those consisting of several continuum solid constituents, find wide applicability in engineering, due to their superior mechanical and thermal properties, and lower cost, relative to the individual components. Due to their complex, multiscale microstructures, composites offer a fertile field for researching their macroscopic behavior with respect to various transport processes, including heat transfer. Many different types of composite materials, such as long-fiber-reinforced, short-fiber-reinforced, laminates, and particulate, are used in applications in the aerospace, automobile, electronic and other industries.

The subject of heat transfer in composites is vast. According to Furmański [1], conduction is the most preponderant mode of heat transfer in



such materials. The convection and radiation modes are of importance in special cases, such as when the composite has significant fluid-filled void content (Tzou [2]), or in open-cellular materials (Kamiuto [3]). The determination of the effective thermal conductivity is thus the main goal of innumerable experimental, analytical, and computational approaches to determine the macroscopic thermal behavior of composite materials. In this paper, we are primarily interested in the computational approaches. Depending on the geometric model adopted to represent the composite microstructure, heat conduction can be treated as a one-, two-, or three-dimensional phenomenon.

Many factors affect the effective thermal conductivity of composites. Theoretically, only the temperatures, thermal conductivities, relative volume amounts, geometries, and spatial and size distributions of the constituent phases should play a role. However, because actual manufacturing processes of composite materials often lead to imperfections, in practice the effective conductivity also depends on the interfacial thermal resistance between the phases and the porosity (void) content. Also, analytical and computational analyses become more complicated when one or more phases are anisotropic (with tensorial transport properties), and when there are nearly-touching or touching inclusions (fibers or particles) in the composite. Usually, those analyses implicitly take into account the temperature dependence of the effective conductivity, by considering temperature dependent properties of the individual phases.

The paper is organized as follows. Because computational models and results must be validated against analytical predictions and/or experimental measurements, we refer to some important analytical and experimental studies in sections 2 and 3, respectively. We remark that, to date, there is much uncertainty in determining the microstructure of a real composite material body, and therefore comparison of analytical and numerical results to experimental data remains a difficult task. In section 4, we discuss various computational approaches developed to study heat conduction in composite materials. In section 5, we present sample comparative analyses of representative numerical results, analytical predictions, and experimental measurements. Finally, in section 6, we offer some conclusions.

## 2 Analytical studies

Recent, comprehensive reviews of analytical and experimental techniques for the study of heat conduction in composite materials are presented by Furmański [1], Mirmira [4], and Ayers and Fletcher [5]. Analytical studies seek to replace the heterogeneous composite medium with a homogeneous medium possessing effective properties, by effecting either a one-equation or a two-equation (mixture-model) homogenization procedure (Furmański [1], Auriault [6]). Such studies *require* that the composite microstructure be

prescribed deterministically or through probability distribution functions, and consequently predict either an exact or an ensemble-averaged value for the effective conductivity (Furmański [1,7], O'Brien [8]). Alternatively, statistical bound methods, reviewed by Torquato [9], aim at determining upper and lower bounds for the effective property of interest, while requiring little microstructural information in the form of correlation functions. Bound methods can yield sharp results provided high-order correlation functions are either known, measured, or constructed (Torquato [10]). Phenomenological approaches (Tzou [2], Acrivos and Shaqfeh [11], Tzadka and Schulgasser [12], Hashin [13]) can address relatively more complex problems by introducing heuristic assumptions, which require *a posteriori* validation.

Analytical work on the subject of effective properties of composite materials started a long time ago, with the pioneering works of Maxwell on particulate composites and of Rayleigh on fibrous composites (Furmański [1]). In the latter case, when the fibers are co-oriented, prediction of the longitudinal effective conductivity is afforded by the rule of mixtures (Mirmira [4]), which may overpredict experimental results due to the presence of voids in the actual composite body. Prediction of the transverse effective conductivity is more difficult. Analytical or semi-analytical treatments can be found in Perrins *et al.* [14] and Han and Cosner [15] for two-dimensional (fibrous) ordered composites, in Sangani and Yao [16] for two-dimensional random composites, in Sangani and Acrivos [17], Zick [18], and McPhedran and Mackenzie [19] for three-dimensional (particulate) ordered composites, and in O'Brien [8], Sangani and Yao [20], and Davis [20] for three-dimensional random composites. Some limitations may apply to the analytical and semi-analytical results, such as linear phenomena, dilute volume fractions, and series convergence difficulties at high volume fractions, particularly for higher values of the conductivity of the dispersed phase.

The influence of the interfacial thermal resistance on the effective conductivity of fibrous and particulate composites has been considered in the analytical studies by Cheng and Torquato [22], Auriault and Ene [23], Hasselman and Johnson [24], Chiew and Glandt [25], in the self-consistent modeling of Benveniste [26], and in the Mori-Tanaka mean-field modeling of Mirmira [4]. Mirmira's model [4] deals with transversely aligned and transversely orthotropic fibers, and also accounts for the porosity content of the composite.

### 3 Experimental studies

As Mirmira [4] points out, most of the experimental work on the determination of the macroscopic thermal behavior of composites has focused on epoxy matrices reinforced with fibers with good mechanical, rather than thermal, properties. Literature on effective conductivity measurements of



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composite materials is not abundant, and, for the most part, deals with composites that are not in use today anymore. Mirmira [4] and Ayers and Fletcher [5] review such experimental studies. Modern composite materials for thermal applications are such that the ratio of the thermal conductivities of the individual phases can be very high (well above 100), which poses difficulties to analytical as well as to computational approaches.

The most common methods to measure or infer the effective thermal conductivity of composite bodies are the steady-state hot plate and the flash methods. Mirmira [4] reviewed ten experimental investigations on conduction in fibrous composites, spanning a somewhat narrow range of fiber volume fractions, from 42% to 72%. Mirmira's experiments [4] were carried out on short-fiber composites with fiber volume fractions of 55%, 65%, and 75%; he found that the transverse effective conductivity did not vary significantly with temperature in the range 293–400 K, and that it increased with volume fraction when volume fraction was low, and subsequently decreased (supposedly due to increased interfacial thermal resistance). Experimental studies were also carried out by Hasselman *et al.* [27], Pilling *et al.* [28], Every *et al.* [29], and Bhatt *et al.* [30]. In the latter two, the effect of the interfacial thermal resistance was considered. Every *et al.* [29] and Bhatt *et al.* [30] performed *a posteriori* matching of model-predicted effective conductivity results to experimental measurements, by selecting values of the contact resistance which led to satisfactory agreement with experimental data; such procedure may yield useful information (e.g., optimum particle size) for the design of composite materials. Based on comparisons of his experimental measurements to model predictions, Mirmira [4] adopted a value of  $11348 \text{ W/m}^2 \cdot \text{K}$  for the interfacial thermal conductance.

## 4 Computational approaches

Many computational approaches have been developed for the analysis of heat conduction in composite materials. Relative to analytical studies, computational approaches are better suited to treat complex geometries and nonlinear phenomena; relative to experimental studies, computational approaches offer better control of the microstructure and of the various parameters which influence the effective conductivity. Typically, actual numerical solution of the continuous heat conduction problem in the domain of interest requires three steps: domain geometry and mesh generation, discretization, and solution of the resultant system of algebraic equations. For the first task, when complex geometries are involved, one can resort to third-party commercial or non-commercial software packages. Discretization can be effected in distinct ways, e.g. via finite elements (Cruz and Patera [31], Cruz, Ghaddar and Patera [32], Ghaddar [33], Cruz *et al.* [34], Cruz [35,36], Machado and Cruz [37], Matt [38], Hou and Wu [39], Veyret *et al.* [40], Rolfes and Hammerschmidt [41], Grove [42]), finite differences

(James and Keen [43]), boundary elements (Ingber *et al.* [44]), finite volumes. Solution of the algebraic systems of equations can be tackled using iterative or direct, parallel or serial computational strategies.

In Cruz and Patera [31] and Cruz, Ghaddar and Patera [32], a first-principle parallel computational methodology for the prediction of effective properties and statistical correlation lengths of multicomponent random media is described, which is based upon: (i) a variational hierarchical decomposition procedure which recasts the original multiscale problem as a sequence of three scale-decoupled (sub)problems; (ii) a variational-bound nip-element technique by which microscale models are incorporated into the mesoscale problem; (iii) solution of the resulting mesoscale problem by parallel nested Monte-Carlo and finite-element methods. In the macroscale problem for heat conduction in composites, the effective conductivity of the homogenized medium is supplied (*input*) to the energy equation in order to calculate the bulk heat flow rate of interest. In the mesoscale problem, the effective conductivity is calculated (*output*) by solving an appropriate sequence of periodic-cell problems generated in the Monte-Carlo loop. The finite-element procedure to solve the mesoscale problem suffers from the severe geometric stiffness which arises when treating the distorted domains associated with the presence of very close inclusions. The boundaries of very close inclusions form nip regions that may be hard, or even impossible, to mesh, rendering numerical solutions either prohibitively expensive, due to excessive degrees-of-freedom and ill-conditioning, or hopeless. Ghaddar [33] and Cruz *et al.* [34] solved this microscale problem by developing a variational-bound nip-element methodology to alleviate the difficulties caused by geometric stiffness; they applied the technique to the problem of heat conduction in composites with insulating long fibers. The hybrid analytico-computational methodology is rigorously applicable to problems for which the effective property of interest is the extremum of a quadratic, symmetric, positive-(semi)definite functional. The approach proceeds by an inner-outer decomposition of the geometrically stiff problem, in which analytical approximations in inner nip regions — the microscale models — are folded into a modified outer problem defined over a geometrically more homogeneous domain. As a result, by virtue of the variational nature of the problem, rigorous upper and lower bounds for the configuration effective property may be designed. More recently, in Cruz [35,36], Machado and Cruz [37] and Matt [38], the methodology of Cruz and Patera [31] and Cruz *et al.* [32] has been extended to compute the effective conductivity of two- and three-dimensional ordered composites with a thermally-conducting dispersed phase.

Hou and Wu [39] developed a multiscale finite element method for two-dimensional elliptic problems in heterogeneous media; the method is based on constructing local base functions which capture small-scale effects on the large-scale solution. Their method is parallelizable, and is applicable to both periodic and non-periodic media, and to problems with separable



or continuous scales. Hou and Wu [39] applied their method to solve model elliptic problems in regular geometries, proved convergence of the method, and studied the influence of different boundary conditions for the base functions on the numerical solution. Veyret *et al.* [40] developed a numerical approach, based on the finite element method, to calculate the effective conductivity of granular or fibrous ordered composite materials. They studied composites with and without contacts between inclusions. The influence of contacts between inclusions on the effective conductivity was evaluated by introducing 'thermal bridges,' whose conductivities lay between the values of the phase conductivities. Rolfes and Hammerschmidt [41] calculated the effective conductivity of carbon-fiber-reinforced plastics; the calculations were effected on representative ordered cells, using a commercial finite element package. Grove [42] combined finite element analysis with spatial statistical techniques to determine the transverse thermal conductivity of two-dimensional fibrous composites; his approach was used to generate results for both ordered and random composites.

## 5 Sample Analyses

### 5.1 Ordered composites

Several numerical results are available for the effective thermal conductivity of two- and three-dimensional ordered composites; the most common results are for the square array and hexagonal array of infinite circular cylinders (used as models for long-fiber-reinforced composites), and for cubic arrays of spheres (used as models for particulate composites). Representative results for the square array of cylinders and for the simple cubic array of spheres have been brought together in Tables 1 and 2, respectively, where we show the effective conductivity, nondimensionalized relative to the matrix conductivity, for various values of the concentration (inclusion volume fraction),  $c$ , and the ratio of inclusion to matrix conductivities,  $\alpha$ . In Table 1,  $k_c^P$ ,  $k_c^C$ ,  $k_c^V$  and  $k_c^{RH}$  refer, respectively, to the analytical results of Perrins *et al.* [14], and the numerical results of Cruz [35], Veyret *et al.* [40] (interpolated from the plots in their Figures 4 and 8) and Rolfes and Hammerschmidt [41] (read directly from the plot in their Figure 7); in Table 2,  $k_s^{SA}$ ,  $k_s^C$  and  $k_s^M$  refer, respectively, to the analytical results of Sangani and Acrivos [17], and the numerical results of Cruz [36] and Matt [38]. Cruz [36] obtained his results using linear tetrahedral meshes with nominally uniform mesh spacing; Matt [38] improved the meshes of Cruz [36] by refining them in the gap regions between neighboring spheres. In addition to the results in Table 1, for the concentration  $c = 0.785$  (close to maximum packing, very stiff domain geometry), Machado & Cruz [37] obtain the lower bounds of 1.704 and 13.5, and the upper bounds of 1.723 and 23.3, for  $\alpha$  equal to 2 and 50, respectively; such bounds yield the corresponding effective conductivity estimates of 1.713 and 18. For the same values of  $c$  and  $\alpha$ , Perrins *et al.*

[14] obtain  $k_c^P$  equal to 1.722 and 20.5, respectively. From the exposed results, we can conclude that calculations of the effective conductivity of two- and three-dimensional ordered composites, performed by many different authors, agree very well.

Table 1: Transverse effective conductivity results for the square array of cylinders, for various values of the concentration,  $c$ , and the conductivity ratio,  $\alpha$ .

$c$	$\alpha$					
	2		50			
	$k_c^C$	$k_c^P$	$k_c^C$	$k_c^P$	$k_c^V$	$k_c^{RH}$
0.1	1.069	1.069	1.213	1.213	—	—
0.2	1.143	1.143	1.476	1.476	1.6	—
0.3	1.222	1.222	1.813	1.813	2.0	—
0.4	1.308	1.308	2.263	2.263	2.3	—
0.5	1.401	1.401	2.915	2.915	2.9	2.9
0.6	1.503	1.503	3.990	3.988	4.1	4.0
0.7	1.615	1.615	6.342	6.336	6.3	6.3
0.77	1.702	1.702	12.75	12.74	—	—

Table 2: Effective conductivity results for the simple cubic array of spheres, for various values of the concentration,  $c$ , and the conductivity ratio,  $\alpha$ .

$c$	$\alpha$				
	2		50		
	$k_s^C$	$k_s^{SA}$	$k_s^C$	$k_s^{SA}$	$k_s^M$
0.05	1.038	1.038	1.152	1.148	1.149
0.10	1.076	1.077	1.320	1.312	1.313
0.20	1.157	1.158	1.712	1.702	1.702
0.30	1.243	1.244	2.227	2.200	2.220
0.35	1.288	1.289	2.576	2.564	2.565
0.40	1.334	1.335	3.035	3.008	3.008
0.50	—	1.434	—	4.572	4.572

## 5.2 Three-dimensional short-fiber composites

In the recent study by Matt [38], the three-dimensional microstructural model of a periodic cell composed of a short circular cylinder placed at the geometric center of a cubic matrix and along one of its horizontal axis, was chosen to represent short-fiber-reinforced composites. Inside the cell volume, Matt [38] generated simple linear tetrahedral meshes with nominally



uniform mesh spacing. Based on the data of Mirmira and Fletcher [45] for a certain type of composite material with short fibers dispersed in an organic matrix, Matt [38] chose the following parameters for his computations: ratio of fiber diameter to fiber length equal to 2; ratio of fiber to matrix conductivities equal to 1580. The volume fraction corresponding to maximum packing for the given cell geometry and aspect ratio of 2 is 0.39. The fiber volume fraction,  $c$ , was varied, and the transverse effective conductivity calculated. Matt's [38] and Mirmira and Fletcher's [45] (read directly from the plot in their Figure 2, at temperature 450 K) results,  $k_{sf}^M$  and  $k_{sf}^{MF}$ , respectively, are presented in Table 3. It is observed that while Matt's results increase with increased volume fraction, Mirmira and Fletcher's results decrease. Also, the maximum volume fraction that Matt can possibly simulate is less than the volume fractions of the actual composite bodies. Clearly, Matt's simple model for the microstructure is not appropriate to represent Mirmira and Fletcher's composites; also, Matt did not account for the influence of the interfacial thermal resistance on the transverse effective conductivity. We can therefore conclude that more sophisticated geometric and physical modeling need to be incorporated into computational approaches for conduction in short-fiber composites. It should also be pointed out that experimental results for values of  $c$  lower than 0.55 are of interest to aid comparisons between numerical and experimental results.

Table 3: Matt's numerical [38] and Mirmira and Fletcher's [45] experimental results for the transverse effective conductivity of short-fiber composites.

$c$	$k_{sf}^M$	$k_{sf}^{MF}$
0.10	1.55	—
0.15	1.90	—
0.20	2.35	—
0.25	3.01	—
0.30	4.03	—
0.55	—	4.20
0.65	—	4.00
0.75	—	3.00

### 5.3 Random composites

Few numerical results are available for the effective conductivity of two- and three-dimensional random composites. In Cruz and Patera [31], results are presented for random composites with insulating long fibers ( $\alpha = 0$ ), for the concentrations  $c \in \{0.1, 0.2, 0.3, 0.4, 0.5\}$ . Grove [42] presents results for random composites with conducting long fibers, for the ranges  $0.05 \leq$





$c \leq 0.5$  and  $2 \leq \alpha \leq 500$ . Sangani and Yao [16] present semi-analytical results for random composites with long fibers for  $c \in \{0.1, 0.3, 0.5, 0.7\}$  and  $1 \leq \alpha \leq \infty$ . Because different statistical models and sample sizes are used in these studies, comparisons between their results are not immediate. No comparisons with experimental results of the numerical results obtained by Cruz and Patera [31] and Grove [42], and of the semi-analytical results obtained by Sangani and Yao [16] are presented.

## 6 Conclusions

We have described several computational approaches for the study of heat conduction in composite materials. It has been pointed out that, while a vast body of results exists for the effective conductivity of two- and three-dimensional ordered composites, none of the computational approaches has been extensively used to generate benchmark results for the effective conductivity of random (disordered) composites. Also, none of those approaches takes into account the presence of porosity in the composite. Finally, we remark that further developments are needed in the geometric and physical modeling of three-dimensional heat conduction in composite materials, so that computational approaches can yield more realistic results.

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