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Predicting the effective thermal conductivities of composite materials and porous media by machine learning methods

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ABSTRACT

Composite materials have a wide range of engineering applications, and their effective thermal conductivities are important thermo-physical properties for real applications. The traditional methods to study effective thermal conductivities of composite materials, such as the effective medium theory, the direct solution of heat diffusion equation, or the Boltzmann transport equation, are all based on developing good physical understanding of heat transfer mechanisms in those composite materials. In this work, we take a completely different approach to predict the effective thermal conductivities of composite materials using machine learning methods. With a set of trustable data, the support vector regression (SVR), Gaussian process regression (GPR) and convolution neural network (CNN) are employed to train models that can predict the effective thermal conductivities of composite materials. We find that the models obtained from SVR, GPR, and CNN all have a better performance than the Maxwell-Eucken model and the Bruggeman model in terms of predicting accuracy. Our work demonstrates that machine learning methods are useful tools to fast predict the effective thermal conductivities of composite materials and porous media if the training data set is available. The machine learning approach also has the potential to be generalized and applied to study other physical properties of composite materials.

1. Introduction

Composite materials and porous media have wide engineering applications, e.g., automobile industries and aeronautical applications like components of rockets, aircrafts, etc. [1,2]. The effective thermal conductivity is one of the most significant thermo-physical characteristics of the composite material. To predict the effective thermal conductivities of composite materials, the factors, including the thermal conductivity, size, and distribution of the inclusion, that may affect the effective thermal conductivities should be considered [3].

There are numerous existing methods, such as effective medium theory (EMT) [4–6], the direct solution of heat diffusion equation [7], and the solution of Boltzmann transport equation (BTE) [8] to predict the effective thermal conductivities of composite materials and porous media. The EMT [9] provides simple analytical models that can quickly estimate the effective thermal conductivities of the composite materials [10], knowing the properties and volume fractions of the inclusions. For example, Maxwell [11] was the first person to give analytical expressions for effective thermal conductivities of composite materials. The Maxwell model considers dilute dispersion of spherical particles embedded in a continuous matrix, where thermal interactions between inclusions are ignored. To consider the thermal interactions, the Bruggeman model [12] has been developed and it is considered to be more accurate for high filler volume fractions. EMT is simple but the accuracy is limited because it does not consider the effect of the distribution of inclusions. To consider the details of materials distribution in a composite, direct solutions of heat diffusion equation are generally adopted. Many numerical methods are developed to solve the equation, such as finite volume method (FVM) [13] and the finite element method (FEM) [7]. Other methods, such as the lattice Boltzmann method (LBM) [14,15], have also been developed to calculate the effective thermal conductivity at sub-continuum scale by solving BTE [8,16]. All these approaches are based on physical modeling, i.e., solving partial differential equations (PDE), which generally requires a high computational cost. On the other hand, experiments can always be carried out to study the heat transfer in composite materials [17]. The issues include the cost of experiments and uncertainties in the measurements.

With the rapid development of machine learning methods recently [18], there has been a growing interest to develop surrogate models to solve engineering problems based on data analysis while bypassing the detailed understanding of the physical

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Nomenclature

D	training data set
$\mathbf{x}_i$	vectors of descriptors
y_i	objective value
$\mathbf{w}$	weight vector
b	bias
C	penalty factor
k_1 (W/mK)	thermal conductivity of matrix
k_2 (W/mK)	thermal conductivity of inclusion
v_2	volume fraction of inclusion
k (W/mK)	effective thermal conductivity
c_d	core distribution probability
D_i	directional growth probability
t (s)	real time
$(\rho c_p)_m$	volume thermal capacity of matrix
$(\rho c_p)_i$	volume thermal capacity of inclusion
p	volume fraction of growing phase
r	location vector
δt	time step
g_α	evolution variable
g_α^{eq}	equilibrium distribution of g_α
e_α	discrete velocity
c	pseudo sound speed
y_i'	predictive value

Greek symbols

γ	width of the Gaussian function
α_i, α_i^*	Lagrange multiplier
τ	dimensionless relaxation time

mechanism or conducting the experimental measurements. For example, Zhan et al. tried different machine learning models to predict the interface thermal resistance between two materials and found that machine learning methods can be more accurate than the commonly used acoustic mismatch model and diffuse mismatch model [19]. Among the machine learning methods, the support vector regression (SVR) [20–22] is a simple, accurate and reliable model for non-linear regression analysis [23]. Besides the SVR, Gaussian process regression (GPR) [24] is another conventional machine learning method for regression and can be used to solve the non-linear regression problems [25]. Since predicting the effective thermal conductivities of composite materials from various factors is a non-linear regression problem, SVR and GPR can be suitable. In addition to SVR and GPR, the deep learning method using neural network [26,27] has been developing fast and successfully applied to image recognition and object detection as a modern approach of computer vision methods [28,29]. Convolution neural network (CNN) [30,31] has been widely used in face recognition and object detection, and achieved very good accuracy. For the composite materials, it is also necessary to extract structural features and find out the correlation between these structures and the final effective property. Similar to face recognition, CNN can be adopted to capture the features of the microstructure in composite materials.

Based on the considerations above, we propose a framework to use machine learning methods, including SVR, GPR and CNN to study the heat transfer in composite materials and porous media in this work. Machine learning approaches can be regarded as semi-analytical models, and from this perspective it is similar to EMT because it can provide a fast prediction with negligible computational cost. The difference is that EMT is based on physical understanding, but machine learning is based on data analysis. We emphasize that the machine learning approach is a complement (not a replacement) of physical modeling and experimental measurements. It can be regarded as a surrogate model that can provide a fast prediction of a composite material without solving time-consuming PDE or conducting experiments. Such a general idea of extracting information from data has been recently demonstrated in material science community and the importance has been realized [32–34]. To demonstrate the capacity of machine learning methods for heat transfer analysis, we created a database using the quartet structure generation set (QSGS) [16] to generate composite material structure and applying LBM to calculate the effective thermal conductivity. We remark that such a choice of database is not necessary to conduct our machine learning analysis. We choose this method because the data set can be easily obtained for demonstration purpose. The database can also be taken from experimental results or other reliable approaches, but the availability is limited right now. Throughout the manuscript, we regard LBM results as "accurate". This is reasonable because the results obtained from the energy BTE follow the physical laws for heat diffusion in macroscopic composite systems (the sub-continuum effects like interface thermal resistance and size effect are neglected for simplicity). Using these data as the training data set, we applied the SVR model, GPR model, and CNN model to predict the effective thermal conductivity of composite materials. We compared the root mean square error (RMSE) with that of Maxwell-Eucken model and Bruggeman model and showed that they can be more accurate than these EMT models. The advantages and drawbacks of the machine learning approaches are also discussed.

2. Methodology and simulation process

2.1. Support vector regression and Gaussian process regression

SVR and GPR are supervised learning methods for regression analysis [23,24,34,37] that make different assumptions. In terms of studying heat transfer in composite materials, both of them can be used to obtain models to predict effective thermal conductivities (or "objective values") from the distribution and properties of the inclusions (or "descriptors"). The parameters of the models are learned from training data set containing n pieces of data, $D = \{(\mathbf{x}_i, y_i) \mid i = 1, 2\ldots n\}$, among which $\mathbf{x}_i$ are vectors composed of all descriptors and y_i are objective values.

In order to solve non-linear regression problems, SVR maps the input space (variables are the descriptors) into a high dimensional feature space (variables are nonlinear transformation of the descriptors), and then perform linear regression in the feature space [35]. The feature space is determined by kernel functions, so the regression function will be a linear combination of these functions. In our work, we choose the Gaussian function [24], which is also called Radial Basis Function (RBF), as the kernel function:

$$K(\mathbf{x}, \mathbf{x}_i) = \exp\left(-\frac{\|\mathbf{x}-\mathbf{x}_i\|^2}{2\sigma^2}\right) = \exp(-\gamma\|\mathbf{x}-\mathbf{x}_i\|^2), \tag{1}$$

which is commonly used if there is no prior knowledge about the real distribution of the data. The final regression function is