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Optimized Lattice Monte Carlo for thermal analysis of composites

T. Fiedler *, I.V. Belova, A. Rawson, G.E. Murch

Centre for Mass and Thermal Transport in Engineering Materials, The University of Newcastle, Callaghan, NSW 2308, Australia

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ABSTRACT

This paper addresses the use of the Lattice Monte Carlo method for the thermal characterization of composite materials. An optimized approach that minimizes computational time is presented. The key aspect of the approach is the avoidance of the need to model the local thermal inertia. A combined finite element and Lattice Monte Carlo analysis is conducted on a model composite for a formal verification of the effective thermal diffusivity and conductivity calculated by the optimized Lattice Monte Carlo method. The effective thermal inertia is calculated separately by making use of the energy conservation law.

1. Introduction

Since its appearance more than 70 years ago, the Monte Carlo method has undergone numerous developments and has enjoyed applications in virtually every area of science and engineering. The Monte Carlo method has been a popular method for addressing both mass and heat transport problems in materials. For mass transport, the Monte Carlo method has been used for many years for addressing atomistic problems in crystalline solids (in such problems it is now usually called the Kinetic Monte Carlo (KMC) method; see [1] for an early review and [2] for a typical recent KMC calculation). More recently, a lattice-based random walk Monte Carlo method has been used for addressing phenomenological problems (where it has been termed the Lattice Monte Carlo (LMC) method [3,4] to differentiate it from the KMC method). In addressing heat transport problems, the LMC method has been used for investigating transient heat conduction problems in homogeneous materials (where a continuous random walk method has also been used [5]). The LMC analysis has proved to be a very versatile and robust numerical method that can be used to conduct transient thermal simulations as well as to determine effective thermal properties (usually via equilibrium thermal simulations). Recently, the LMC method has been adapted to address these problems in inhomogeneous materials [6,7].

2. Introductory remarks about the methods used

We consider a composite material consisting of n different phases with Φ_i, k_i, c_i, ρ_i, as the volume fraction, thermal conductivity, specific heat and density, respectively, of an individual phase i. The thermal inertia I_i of a phase i is the product $I_i = c_i\ \rho_i$. The thermal inertia of the whole composite I_{eff} then is calculated simply as (see the Appendix for a derivation based on mass balance):

$$I_{eff} = \sum_{i=1}^{n} I_i \Phi_i \tag{1}$$

The thermal diffusivity of each phase i is given by:

$$D_i = \frac{k_i}{c_i \rho_i} \tag{2}$$

and the effective diffusivity D_{eff} of the composite is given by:

$$D_{eff} = \frac{k_{eff}}{I_{eff}} \tag{3}$$

To calculate an effective thermal conductivity k_{eff} and diffusivity D_{eff} for a composite the following methods can be used. First, a steady-state FEA method can be employed. In this, an appropriate *steady-state* temperature distribution is generated and Fourier's law is utilized in order to obtain the effective thermal conductivity. In this type of numerical simulation there is no need for modeling the inertias of the phases in the composite. Making use of Fourier's law, the effective thermal conductivity k_{eff} of the composite can be obtained according to:

* Corresponding author. Tel.: +61 02 4921 6188; fax: +61 02 4921 6946.
E-mail address: Thomas.Fiedler@newcastle.edu.au (T. Fiedler).

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$$k_{eff} = \frac{dQ}{dt} \cdot \frac{\Delta x}{\Delta T \cdot A} = \frac{dQ}{dt} \cdot \frac{1}{\Delta T \cdot \Delta x}, \quad (4)$$

where dQ/dt is the resulting constant heat flux, Δx is the side length of the unit cell and $A = \Delta x^2$ is the control surface. As stated above, the effective thermal diffusivity of the composite can then be determined using Eq. (3).

A transient FEA method is possible and consists of the calculation of the time-dependent temperature profile for the geometry where an exact analytical solution is available [8]. Then, fitting the exact solution to the profile, in principle, should give the effective thermal diffusivity. Obviously, implementation of this method requires modeling of the thermal inertia of each phase.

Another possible method is an analytical approach. Depending on the geometry of the phases in the composite there are several suitable analytical formulae to determine the effective thermal conductivity. Though approximate, they usually provide useful insight into the structure of the effective thermal properties. We consider here the Maxwell [9] relation for the effective thermal conductivity. This relation gives the best results when applied to a composite with one matrix phase and the remaining *n-1* phases are distributed as inclusions. The inclusions should be well separated from each other. Derivation of this type of relation was made in [10] and the effective thermal conductivity then is given as:

$$k_{eff,Maxwell} = k_1 \left(1 + 2\sum_{j=2}^{n} \Phi_j \frac{k_j - k_1}{k_j + 2k_1}\right)\left(1 - \sum_{j=2}^{n} \Phi_j \frac{k_j - k_1}{k_j + 2k_1}\right)^{-1}. \quad (5)$$

To transform this relation into the relation for the thermal diffusivity, we use Eq. (3), which was first derived in [11,12]:

$$D_{eff,Maxwell} = \frac{k_{eff,Maxwell}}{I_{eff}} = k_1 \left(1 + 2\sum_{j=2}^{n} \Phi_j \frac{k_j - k_1}{k_j + 2k_1}\right)\left(I_{eff}\left(1 - \sum_{j=2}^{n} \Phi_j \frac{k_j - k_1}{k_j + 2k_1}\right)\right)^{-1}. \quad (6)$$

Both steady-state FEA and analytical approaches clearly and correctly show that the effective thermal conductivity does not depend on the thermal inertias of the individual phases. This fact can be taken advantage of when the equilibrium LMC method is employed for the calculation of the effective thermal conductivities and diffusivities. This is precisely the reason for the introduction of an *optimized* LMC method which has been given previously only in the form of a recipe [8]. Here, in order to validate this approach, steady-state and transient FEA methods in parallel with the *full* and *optimized* LMCs are performed for a series of test simulations for a model composite structure. In addition, an analytical (approximate) Maxwell relation is used for calculation of the effective thermal properties.

As mentioned above, the effective thermal conductivity can be calculated using analytical, finite element or Lattice Monte Carlo methods. Analytical methods allow for fast calculations; however, they are mostly limited to simple geometries and merely provide estimates for more complex structures. Finite element analysis is a powerful method for thermal conductivity calculations. Limitations are a possible mesh dependence of the solution and the restriction to only determination of a single direction conductivity per simulation. The generation of the calculation model (i.e. the finite element mesh) requires expertise for ensuring numerical convergence and accurate geometric representation. On the other hand, Lattice Monte Carlo analysis computes the complete thermal conductivity/diffusivity tensor in a single simulation. Furthermore, a simple voxel calculation model can be used when data are drawn from a micro-computed tomography image. On the downside, a single LMC calculation requires coding by the user and typically more computation time than a corresponding finite element simulation. However, this is balanced by the computation of the complete conductivity tensor and reduced modeling time.

2.1. Lattice Monte Carlo algorithm

In the implementation of LMC, the simulation traces the displacements of the probing (energy) particles within a system at thermal equilibrium (i.e. a uniform temperature). To distinguish it from the transient LMC simulation that calculates time-dependent temperature profiles [13] it can also be called an equilibrium LMC. It should be mentioned here that there is no experimental analogue to this approach. However, in the very closely related field of mass diffusion the vector displacements $\boldsymbol{R}$ in time t of single atoms can be traced to calculate their mass diffusivity according to the Einstein equation [14,15] in d dimensions ($d = 1, 2, 3$):

$$D = \frac{\langle R^2 \rangle}{2dt}, \quad (7)$$

where the Dirac brackets $\langle\,\rangle$ indicate an average over a large number of atoms. In a LMC simulation of thermal transport, energy particles are injected into the geometric model (the lattice) and permitted to explore its structure via random walks. These lattice-based random walks are directed by selection and jump probabilities that contain the material model of the simulation.

In general, any LMC algorithm has three sequential stages: initialization, calculation and evaluation. First, let us consider initialization for the *full* LMC. In this stage, the geometry and thermal properties of the constituent phases, thermal conductivity k_i and thermal inertia I_i are all defined. The geometry is represented by a lattice model that is assembled by nodes. Each node represents a control volume and is located at its center. Corresponding to the target geometry the material properties are assigned to each volume/lattice node. The easiest lattice structure for the arrangement of the nodes is a simple cubic one, but other lattices may be selected if required. Next, energy particles are distributed within the lattice (multiple occupancy of a node is possible). For an equilibrium LMC simulation a constant temperature is required throughout the composite. To this end, each equal-sized control volume V is represented by its lattice node and is populated with energy particles. The amount of energy E_i required per lattice node for a constant temperature T throughout a composite can be calculated according to:

$$E_i = T \cdot V \cdot \rho_i \cdot C_i = T \cdot V \cdot I_i. \quad (8)$$

Therefore, Eq. (8) dictates that energy particles are not evenly distributed but must be segregated according to the thermal inertia I_i of each phase. The constant energy content of a particle is the system energy $\sum E_i$ divided by the total number of particles. The number of particles can be chosen freely; a higher number of particles improves numerical accuracy (according to the Central Limit Theorem and with the relative error being inversely proportional to the square root of the number of particles) but simultaneously of course increases the simulation time.

In LMC simulations the energy particles are permitted to explore the structure on random walks. Walks are random insofar as the jump direction is chosen randomly. For example, in a three-dimensional simple cubic model, a total of six jump directions (i.e. positive and negative x, y and z directions) are possible. At the beginning of each jump attempt, the LMC simulation time t_{LMC} is incremented by one time step. In the *full* LMC a successful jump from a node to its nearest neighbor requires overcoming both the selection and jump probabilities. The selection probability implements the thermal inertia and maintains particle segregation (i.e. a uniform temperature) in the LMC model. The selection