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A mesh-free Monte-Carlo method for simulation of three-dimensional transient heat conduction in a composite layered material with temperature dependent thermal properties

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ABSTRACT

A new solution for the three-dimensional transient heat conduction from a homogeneous medium to a non-homogeneous multi-layered composite material with temperature dependent thermal properties using a mesh-free Monte-Carlo method is proposed. The novel contributions include a new algorithm to account for the impact of thermal diffusivities from source to sink in the calculation of the particles' step length (particles are represented as bundles of energy emitted from each source), and a derivation of the three-dimensional peripheral integration to account for the influence of material properties around the sink on its temperature. Simulations developed using the proposed method are compared against both experimental measurements and results from a finite element simulation.

1. Introduction

The Monte-Carlo method (MCM) is prominent for its ability to tackle complex simulation problems based on random number generation. Numerical solutions based on finite difference and finite element methods have been conventionally adopted for solving multi-dimensional heat conduction problems, although some issues remain problematic with these approaches. For instance, the stability criterion in the explicit finite difference method limits the time step to the grid size. Implicit approaches [1] are used in the majority of linear solvers and FEM packages due to their numerical stability. Implicit applications convert the problem's geometry to a grid of small elements that lead to a matrix that must be solved by inversion to obtain the result at each time increment. Complex geometries that require small grid size lead to large matrices and therefore larger computational and memory requirements: inversion of large assembly matrices is time consuming. This becomes a significant practical consideration in problems with complex geometries and Multiphysics problems [2]. By contrast, Monte-Carlo methods have significant advantages relative to these methods [3]. First, there is no requirement to build an assembly matrix and consequently no need for matrix inversion. Second, the solution at a desired point in the domain can be obtained independently from the solutions at other points within the domain. These features lead to a significant reduction in simulation time by solving for specific regions of interest, instead of solving for the entire domain, which requires inversion of the entire assembly matrix. Inverse heat conduction (the prediction of surface temperature and heat flux using the time history of temperature at internal points in the domain) is another important problem that benefits from this feature [4]. Third, the Monte-Carlo approach is stable and very well suited for parallel computing, which is particularly attractive with the advent of GPU engines [2]. Apart from the aforementioned general advantages, using random parameters in MCM makes it a powerful approach to model problems with inherited random or stochastic behaviors or parameters. For instance porosity in porous media can be defined as a random parameter [5–9], making MCM an excellent option for simulation.

The Monte-Carlo method was first described in 1949 [10] by Metropolis and Ulam as a statistical approach for solving integro-differential equations. In heat conduction, Haji-Sheikh and Sparrow [11] described the application of MCM to solve heat

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conduction problems with homogenous isotropic material properties for different types of boundary conditions. Other studies have used [11] to develop methods to solve conduction heat transfer problems where thermal properties are not isotropic, as in composite layered materials. The fixed random walk MCM was modified [12,13] to solve transient heat conduction in anisotropic media. The necessity of a grid to define the geometry is a disadvantage of the fixed random walk method, compared to floating random walk. Non-homogeneity of thermal properties in a heat conduction domain has been shown in [14] by relating the impact of the non-homogeneity on the temperature distribution in proportion to the thermal diffusivity of source and sink. In cases with abrupt changes in thermal diffusivity, such as at cryogenic temperatures or in composite layered materials, the aforementioned approach of proportion leads to significant error. This paper presents a novel solution for transient heat conduction in anisotropic materials with abrupt changes in thermal diffusivity based on MCM.

2. Formulation

Heat transfer process describes the transmission of an energy bundle (particle in this study) from source to sink. In a reverse approach, one can use the known thermal properties of the sink to estimate the sources that can transfer energy to the sink in a corresponding time span. The domain is filled with K uniformly generated points that represent sinks with known initial conditions that define the temperature at each point. The solution process starts by emitting J particles from each sink to find the location of the sources, which could be anywhere within or beyond the boundaries of the domain and not necessarily on the sink locations. If the source location falls inside the domain, the temperature at that location can be interpolated using the known temperatures of neighboring points from the previous time step. The scattered interpolation uses four closest neighboring points. Otherwise, the following boundary conditions apply for particles falling on or outside of boundaries at each time step. First, a fixed temperature boundary condition: particles adopt the pre-assigned fixed temperature of the boundary. Second: Insulation boundary condition: particles adopt the temperature of the sink. Third: convection boundary condition, has not been considered in this paper. Other studies [15,16] have proposed methods for taking the convective boundary condition into account. Three-dimensional conductive heat transfer in a domain with homogeneous thermal diffusivity (as described in [11]) presents the method to estimate source locations. From the three dimensional heat conduction relation in spherical coordinates ([17,18]) one can find the temperature at the sphere's center as:

$$T(x,y,z,t) = \int_{F=0}^{1}\int_{G=0}^{1}\int_{\tau=0}^{t} T(r,\varphi,\theta,t-\tau)\,dF\,dG\,dH^{(3)} \tag{1}$$

$$F(\varphi) = \frac{\varphi}{2\pi} \tag{2}$$

$$G(\theta) = \frac{1}{2}(1-cos\theta) \tag{3}$$

$$H^{(3)}\left(\frac{\alpha\tau}{r^2}\right) = 1 + 2\sum_{k=1}^{\infty}(-1)^k \exp\left(\frac{-k^2\pi^2\alpha\tau}{r^2}\right) \tag{4}$$

Eq. (1) illustrates the integral form for the temperature at the sphere's center based on the known temperature of particles emitted from its vicinity. Eqs. (2) and (3) describe the probability functions of angles θ and φ, respectively. The time step τ and steplength r of each floating random walk are related to the thermal diffusivity α at each point by the probability function (4): the higher the thermal diffusivity, the longer the step length (or the shorter the required time step). The inverse functions for Eqs. (2)–(4) [19] are: Eq. (7) is obtained from a fit function on inverse of Eq. (4).

$$\varphi = 2\pi(RN_1) \tag{5}$$

$$\theta = cos^{-1}[1-2(RN_2)] \tag{6}$$

$$\begin{aligned} \frac{\alpha\tau}{r^2} &= D_1 + D_2(RN_3) + D_3(RN_3)^2 + D_4(RN_3)^3 \quad RN3 < 0.6 \\ \frac{\alpha\tau}{r^2} &= -0.10132ln[0.5(1-RN_3)] \quad RN3 \geqslant 0.6 \end{aligned} \tag{7}$$

RN in Eqs. (5)–(7) denotes uniform random numbers generated from a Halton sequence (uniformly distributed random numbers) in three different sets. Table 1 shows the values of the D coefficients in these equations [19].

Fig. 1 depicts the inverse of the probability function $H^{(3)}$, where the random number RN_3 from the Halton sequence is the abscissa and the ordinate value is $\frac{\alpha\tau}{r^2}$. With the known thermal diffusivity of sink α and time step τ, the steplength r can be calculated.

By calculating the angles and steplength as described above, one can calculate the location of the source using Eq. (8). Once the source location is defined, the temperature at that location is allocated to the particle emitted from the respective source. The sink's temperature is simply the average of the temperature of particles as shown in Eq. (9), where j is the index for the particle number of J particles, t the time step and k the index for point number out of a total of K points [11]:

$$\begin{aligned} x_j &= x_k + r_j \sin(\theta_j)\cos(\varphi_j) \\ y_j &= y_k + r_j \sin(\theta_j)\sin(\varphi_j) \\ z_j &= z_k + r_j \sin(\theta_j) \end{aligned} \tag{8}$$

$$T^{t+1}_{(x_k,y_k)} = \frac{1}{J}\sum_{j=1}^{J} T^{t}_{(x_j,y_j)} \tag{9}$$

Fig. 2 depicts $J = 20$ particles emitted from the source and absorbed by the sink at the center of the sphere. The location of the sources is calculated using the aforementioned approach.

The above equations cover the solution of diffusion problems in homogenous media. Tackling problems in non-homogenous media needs further modifications. First, the thermal diffusivity of and between the source and the sink are not equal; therefore, the steplength calculated from the sink using its thermal diffusivity will not be equal to the steplength calculated from the source using its diffusivity. This affects the reversibility of the particle transport described before: reversibility is not valid in non-homogenous media.

A new algorithm is needed that takes into account the change in thermal diffusivity between source and sink. One approach is to take very small time steps, leading to steplengths small enough to approximate the thermal diffusivity of source and sink as equal. This has some disadvantages: assuming equal thermal diffusivity introduces error, and the approximation is not applicable close to the boundaries in composite layered materials, where thermal diffusivity experiences an abrupt change. Also, acquiring results for desired times requires more iterations due to the smaller time steps, which increases simulation time.

Knowing the thermal diffusivity function enables methods to address the aforementioned issue for non-homogenous media [20,21]; however this may lead to error in case of sharp changes in diffusivity due to the use of derivatives. Refs. [22] shows the required modifications to the two-dimensional Monte-Carlo transient heat conduction equations in cylindrical coordinates that lead