Journal of Computational Physics 265 (2014) 71–96

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Peridynamic thermal diffusion

Selda Oterkus [a], Erdogan Madenci [a,*], Abigail Agwai [b]

[a] Department of Aerospace and Mechanical Engineering, The University of Arizona, Tucson, AZ 85721, USA
[b] Intel Corporation, Chandler, AZ 85226, USA

ARTICLE INFO

Article history:
Received 20 May 2013
Received in revised form 10 January 2014
Accepted 18 January 2014
Available online 6 February 2014

Keywords:
Thermal
Conduction
Diffusion
Peridynamics
Nonlocal

ABSTRACT

This study presents the derivation of ordinary state-based peridynamic heat conduction equation based on the Lagrangian formalism. The peridynamic heat conduction parameters are related to those of the classical theory. An explicit time stepping scheme is adopted for numerical solution of various benchmark problems with known solutions. It paves the way for applying the peridynamic theory to other physical fields such as neutronic diffusion and electrical potential distribution.

1. Introduction

Nonlocal theories have been used to some extent to describe heat conduction on a continuum level. In heat conduction, the thermal energy is transported through phonons, lattice vibration, and electrons. Usually, electrons are the vehicles through which thermal energy is transported in metals while phonons are the heat carriers in insulator and semiconductors. This process of thermal energy transfer is inherently nonlocal because the carriers arrive at one point having brought thermal energy from another. Nevertheless, macroscale heat transfer models that adopt a local formulation, typically employing the Fourier law as the local constitutive relation, have been used successfully to represent continuum heat conduction.

The mean free path of the heat carriers is the average distance a carrier travels before its excess energy is lost. As the heat carriers' mean free path becomes comparable to the characteristic lengths; the nonlocality needs to be taken into account in the continuum model. Nonlocality often becomes important at low temperatures, as exhibited in cryogenics systems, since the heat carriers have a longer mean free path at lower temperatures. It has been found that nonlocality should also be accounted for in problems in which the temperature gradients are steep. This is because the penetration depth, the length characterizing the temperature gradient, becomes short, even becoming of the same order of magnitude as the mean free path of the carrier. In such instances, it is necessary to consider the nonlocality of the heat transport in a continuum model. Recently, with the miniaturization of devices, the small geometric length scales have also necessitated the inclusion of nonlocal effects in microscale and nanoscale models [1].

Several nonlocal heat conduction theories have been proposed in the last few decades. In the early 1980s, Luciani et al. [2] developed a nonlocal theory to better represent electron heat transport down a steep temperature gradient by introducing a nonlocal expression for the heat flux. The nonlocal model was in better agreement with probabilistic simulations (Fokker–Planck simulations) than the local models. Later, Mahan and Claro [3] proposed a nonlocal relation between the heat

* Corresponding author. Tel.: +1 520 621 6113; fax: +1 520 621 8191.
E-mail address: madenci@email.arizona.edu (E. Madenci).

http://dx.doi.org/10.1016/j.jcp.2014.01.027
0021-9991/

current, determined from Boltzmann's equation, and the temperature gradient. In the 1990s, Sobolev [4] introduced a model in which both space and time nonlocality are taken into account in the strong form, i.e. integral form, of the energy balance, Gibbs and entropy balance equations. Lebon and Grmela [5], proposed a weakly nonlocal model (weakly nonlocal models are typically based on gradient formulation). The model was based on nonequilibrium thermodynamics, for which an extra variable is added to the basic state variables to account for nonlocality. Subsequently, they extended their model to include nonlinearity [6]. More recently, the development of nonlocal heat conduction equations has been motivated by the miniaturization of devices. A number of researchers have put forth nonlocal models with the objective of capturing heat transport in microscale and nanoscale devices. One example of this is the ballistic-diffusive heat equation by Chen [7], which was derived from the Boltzmann equation, and it accounts for nonlocality in heat transport. Another example is by Alvarez and Jou [8]. They developed their model by including nonlocal (and memory/lag) effects in irreversible thermodynamics. Tzou and Guo [9] constructed their model by incorporating a nonlocal (and lag) term into the Fourier law.

An area of interest is determining the temperature field in the presence of emerging discontinuities. One class of problems that contains a discontinuity is the heat transfer process which involves phase change such as solidification and melting [10]. This process is commonly referred to as the Stefan problem, and there are a number of technologically important problems that involve heat transfer with phase change. Examples of these include ablation of space vehicles during reentry and casting of metals. Another heat conduction problem with an emerging discontinuity is the rewetting problem from the nuclear industry. Rewetting in a nuclear reactor is employed to restore temperatures to a safe range following accidental dry out or loss of coolant. Emergency cooling is introduced to the system via an upward moving water front or by spraying from the top of the reactor [11,12]. A moving discontinuity occurs in the heat generating solid at the quench front due to the sudden change in heat transfer condition at the solid surface.

Peridynamics is a nonlocal continuum theory which allows governing field equations to be applicable at discontinuities. This applicability at discontinuities is achieved by replacing the spatial derivatives, which lose meaning at discontinuities, with integrals that are valid regardless of the existence of a discontinuity. A peridynamic heat conduction model allows problems with discontinuities are readily solvable as no spatial derivatives appear in the formulation, making the equation applicable everywhere in the body.

The peridynamic theory was initially developed as a reformulation of the equation of motion in solid mechanics that was better suited for modeling bodies with discontinuities, such as cracks [13]. The theory was formulated in what is now referred as the bond-based peridynamic theory, in which a body assumed to be comprised of a network of independent pairwise interactions. However, the independence of the pairwise interactions in solid mechanics leads to certain material limitation. As a result, Silling et al. [14] and Silling and Lehoucq [15] developed a generalized approach to peridynamics in which interactions are not independent, and referred to as state-based peridynamics. Peridynamic states were introduced as the mathematical objects that convey the information associated with a body. Within the realm of solid mechanics, the peridynamic theory has been successfully employed to model fracture nucleation and propagation [16].

A peridynamic approach to heat conduction is advantageous as it not only accounts for nonlocality but it also allows for the determination of the temperature field in spite of discontinuities. The peridynamic heat conduction model is a continuum model; it is not a discrete model. As such the phonon and electron motion is not explicitly modeled. Initial successful attempts have recently been made to develop heat conduction equations in the peridynamic framework. Gerstle et al. [17] developed a peridynamic model for electromigration that accounts for heat conduction in a one dimensional body. Additionally, Bobaru and Duangpanya [18] proposed a one dimensional peridynamic heat conduction equation. Recently, Bobaru and Duangpanya also solved the 2-D heat conduction problem with discontinuities [19]. Both studies adopted the bond-based peridynamic approach.

As part of this study, the heat conduction equation is formulated within the framework of generalized state-based peridynamics. To begin with the peridynamic states are reviewed. The derivation of the generalized peridynamic heat equation is demonstrated using the Lagrangian formalism and the peridynamic variables are explained. Subsequently, simplifications are made to develop the bond-based peridynamic approach for heat conduction from the generalized state-based. The thermal response function and an approach for determining the microconductivity are also presented. A numerical procedure is described for solving the peridynamic heat conduction equations along with the discretization and time stepping schemes as well as numerical stability criterion. Various problems are simulated based upon the present peridynamic heat transfer model, and comparisons against classical solutions are presented in order to establish its validity.

2. State-based peridynamic thermal diffusion equation

Within the peridynamic framework, the interaction between material points is nonlocal. For thermal diffusion, the nonlocal interaction between material points is due to the exchange of heat energy. Therefore, a material point will exchange heat with points within its neighborhood defined by the horizon.

In the Lagrangian formalism, the governing heat conduction equation corresponds to the Euler–Lagrange equation. The Euler–Lagrange equation based on the Lagrangian, L is given in the following form [20]

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\Theta}}\right) - \frac{\partial L}{\partial \Theta} = 0, \tag{1a}$$

with