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A nonlocal Fourier's law and its application to the heat conduction of one-dimensional and two-dimensional thermal lattices

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ABSTRACT

This study focuses on heat conduction in unidimensional lattices also known as microstructured rods. The lattice thermal properties can be representative of concentrated thermal interface phases in one-dimensional segmented rods. The exact solution of the linear time-dependent spatial difference equation associated with the lattice problem is presented for some given initial and boundary conditions. This exact solution is compared to the quasicontinuum approximation built by continualization of the lattice equations. A rational-based asymptotic expansion of the pseudo-differential problem leads to an equivalent nonlocal-type Fourier's law. The differential nonlocal Fourier's law is analysed with respect to thermodynamic models available in the literature, such as the Guyer–Krumhansl-type equation. The length scale of the nonlocal heat law is calibrated with respect to the lattice spacing. An error analysis is conducted for quantifying the efficiency of the nonlocal model to capture the lattice evolution problem, as compared to the local model. The propagation of error with the nonlocal model is much slower than that in its local counterpart. A two-dimensional thermal lattice is also considered and approximated by a two-dimensional nonlocal heat problem. It is shown that nonlocal and continualized heat equations both approximate efficiently the two-dimensional thermal lattice response. These extended continuous heat models are shown to be good candidates for approximating the heat transfer behaviour of microstructured rods or membranes.

1. Introduction

This paper deals with a nonlocal generalization of the heat equation that can be based on lattice arguments. Such nonlocal theories may be useful to capture the scale effects of microstructured solids, when the discreteness at a subscale may play a predominant role at a larger scale. Such scale effects have been experimentally or numerically (based on molecular dynamics simulations) observed, for small scale structures, where size-dependent thermo-mechanical behaviour is noticed. Although the paper is mainly focused on thermal diffusion, fluid infiltration in porous media or electrical conductivity may

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be considered as alternative basic diffusion problems [1]. Nonlocal thermomechanics has been developed since the 1960s based on well-founded thermodynamic arguments [2]. Eringen and Kim [3] or Eringen [4] calibrated the nonlocal elasticity kernel (uncoupled mechanical problem) from lattice mechanics. Lattice mechanics is typically governed by discrete equations, whereas continuum models are known to be better suited for engineering applications, with some more mathematical available framework. There is a need to develop some continuous models which possess some information of the lattice ones. In that spirit, Collins [5] introduced the concept of quasicontinuum to representing a transition medium between the discrete lattice and the asymptotic local continuum. Collins [5] defined this quasicontinuum for a mechanical lattice, with specific application to the soliton phenomenon (see also [6,7]). Rosenau [8] obtained a nonlocal wave equation by continualization of the discrete wave equation. This nonlocal wave equation can be shown to be cast as a differential-based nonlocal model [4], also called a stress-gradient nonlocal model. More recently, the source of nonlocality has been investigated, especially with respect to the inherent microstructure, and in particular for uncoupled mechanical problems (see, recently, [9–11] for nonlocal elasticity problems). Challamel et al. [12] also showed the key role of different microstructures, namely a concentrated or some distributed microstructures. Nonlocal mechanics may be used for characterizing the behaviour of the quasicontinuum. To the authors' knowledge, this methodology has not yet been applied to the thermal analysis of the lattice, so the main aim of this paper is to fill this gap.

It has been demonstrated that the nonlocal kernel for elasticity problems may be related to the discreteness of the material at a fine scale, using a nonlocal differential model introduced by Eringen [4]:

$$\sigma - l_c^2 \sigma'' = E\varepsilon \quad \text{with } \varepsilon = u' \tag{1}$$

where σ is the uniaxial stress, ε is the uniaxial strain, u is the axial displacement, E is the Young modulus, and l_c is a characteristic length which accounts for the specific lattice effect of the equivalent quasicontinuum. For axial vibrations problems, Challamel et al. [11] showed that the length scale of the nonlocal model can be calibrated from the lattice spacing a using:

$$l_c^2 = \frac{a^2}{12} \tag{2}$$

This value is slightly different from the one calibrated by Eringen [4] by comparing the wave dispersive properties of the nonlocal model with the lattice one, also referred to as the Born–Kármán lattice model.

In this paper, we adopt the same methodology used and applied in a one-dimensional problem of thermal diffusion evolution. Nonlocal heat equations have been recently considered using space-fractional derivative operators instead of integer derivative ones [13–17]. In these approaches, the attenuation functions can be introduced by fractional derivative theory, leading to equivalent fractional power law decaying functions. Atanackovic et al. [13] considered a generalized fractional heat equation (also called fractional Cattaneo-type equation) (from the initial work of Cattaneo [18] – see also [19]) with both space- and time-fractional operators, and presented some numerical and analytical solutions. Some more general results including existence and uniqueness properties of Cattaneo-type space–time fractional heat equation (and nonlocal wave-type equations) are available in the books of Atanackovic et al. [20,21]. Michelitsch et al. [14] studied nonlocal wave propagation and nonlocal diffusion processes for self-similar harmonic interactions media using fractional derivatives. Sapora et al. [15] investigated a spatially nonlocal heat equation involving space-fractional derivative operators. Michelitsch et al. [14], Tarasov [16] or Zingales [17] built some space-fractional derivative nonlocal heat equations from a lattice model. Michelitsch et al. [14] or Tarasov [16] considered long-range lattice interactions (nearest-neighbour ones, but also interactions including some other neighbouring) for the physical justification of fractionality, whereas Zingales [17] investigated only nearest-neighbour interactions with power-law lattice non-uniformity. Deseri and Zingales [22] considered a time-fractional Darcy equation (diffusion equation), which can be also considered as a kind of generalized Cattaneo-type equation. Yu et al. [23] coupled Eringen's nonlocal elasticity (integer order spatial differential model) with time-fractional order derivative for the heat conduction. Challamel et al. [9] analytically studied wave propagation in a nonlocal fractional differential-based model, highlighting the possible link between fractional nonlocality and Eringen's differential-based model (see [4] for Eringen's differential model applied to elasticity). Peridynamic heat transfer modelling (which makes use of nonlocal type diffusion equations) has been investigated by Oterkus et al. [24]. Recently, Zhan et al. [25] numerically noticed some length-dependent thermal conductivity in a one-dimensional carbon nanomaterial – diamond nanothread (DNT) – based on non-equilibrium molecular dynamics simulations.

In this paper, we consider an Eringen-type differential model for the nonlocal one-dimensional (and later two-dimensional) generalization of Fourier's law:

$$q - l_c^2 q'' = -\lambda T' \tag{3}$$

where q is the heat flux, T is the temperature, λ is thermal conductivity, and l_c is a characteristic length which contains the microstructure information related to the discreteness of the material. The meaning of this nonlocal parameter is discussed further below. In Eq. (3), we can recognize an Eringen-type nonlocal differential model [4], where the heat flux acts as the stress and the temperature may be associated with the displacement in the analogous case of nonlocal elasticity. Eq. (3) can also be classified as a Guyer–Krumhansl-type equation [26–29], restricted to the nonlocal space contribution as recently highlighted by Sellitto et al. [30], Jou et al. [31] or Jou et al. [32]. The additional nonlocal terms may appear in the kinetic