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Fractional-order theory of heat transport in rigid bodies

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ABSTRACT

The non-local model of heat transfer, used to describe the deviations of the temperature field from the well-known prediction of Fourier/Cattaneo models experienced in complex media, is framed in the context of fractional-order calculus. It has been assumed (Borino et al., 2011 [53], Mongioví and Zingales, 2013 [54]) that thermal energy transport is due to two phenomena: (*i*) A short-range heat flux ruled by a local transport equation; (*ii*) A long-range thermal energy transfer proportional to a distance-decaying function, to the relative temperature and to the product of the interacting masses. The distance-decaying function is assumed in the functional class of the power-law decay of the distance yielding a novel temperature equation in terms of α-order Marchaud fractional-order derivative ($0 \leqslant \alpha \leqslant 1$). Thermodynamical consistency of the model is provided in the context of Clausius–Plank inequality. The effects induced by the boundary conditions on the temperature field are investigated for diffusive as well as ballistic local heat flux. Deviations of the temperature field from the linear distributions in the neighborhood of the thermostated zones of small-scale conductors are qualitatively predicted by the used fractional-order heat transport model, as shown by means of molecular dynamics simulations.

1. Introduction

The need for non-local thermodynamics in physical sciences and engineering may be traced back to the mid of the last century in the attempt to capture the experimental effects unpredicted by Fourier diffusion theory. Indeed several experimental observations of temperature field at metal interfaces as well as of the changes in conductivity parameters in the neighborhood of thermostated regions (Kapitsa phonon-scattering) shows a localization of temperature gradients close to the borders [1].

Similar phenomena have been observed with molecular dynamics (MD) simulations of heat transfer in nanowires showing that the presence of thermostated regions involves a phonon–phonon scattering that modifies the conductivity property of the materials [2,3].

Such studies have been further developed toward the use of advanced mathematical tools as the fractional-order calculus [4] to capture memory [5,6] as well as non-local effects [7–9]. Indeed fractional (real) order integro-differential operators have been introduced more and more often in several contexts of physics and engineering for their capability to interpolate among the well-known integer-order operators of classical differential calculus [10]. In this regard some applications may be

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found in the study of temporal and spatial evolution of complex systems close to critical points [11–14] or in stochastic setting [15–17]. Fractional-order differential calculus is widely used, also, to model the mechanical behavior of polymers, gels, foams and glassy materials [18–22] but also to model the rheology of soft matter and biological tissues [23–25]. States and free energies for non-linear geometries [26–30] in terms of fractional-order derivatives may also be formulated.

The long-tails of fractional operators have been used to formulate non-local stress–strain constitutive equations that are a particularized version of the integral model of non-local elasticity [31,32]. The same feature has been also used by the author and its research team to derive a mechanically-based fractional-order non-local elasticity in statics [33–36] and wave propagation contexts [37,38] (see e.g. [39] for a complete review).

The presence of spatial non-local effects, observed in heat transport framework, has been introduced by means of integral models involving, beside the local gradient of the temperature field, an integral convolution among the temperature gradient and a real-order attenuation function [40–42]. The non-local formulation, originally proposed by Eringen and his co-workers, has been used, recently, to model thermoelastic coupling in microelectromechanical resonators (MEMRS) [43,44]. Some generalization of this theory may be useful to the analysis of small-scale systems accounting for second-sound effects [45–47] modeled with a first-order time derivative of the heat flux [48–50] and introducing a generalized entropy [51,52].

Very recently a non-local model of thermal energy transport has been proposed with a physical picture of heat transfer in 1D setting. It has been assumed that the non-local residual in the balance equation is due to a volume integral over the body domain of the elementary long-range heat transport among adjacent and non-adjacent locations of the body [53]. The long-range thermal energy contribution is modeled as two point function $\mathcal{P}^{(nl)}(\mathbf{x},\mathbf{y},t)$ that depends on: (*i*) A decaying function decreasing with the distance of the interacting elements; (*ii*) The relative temperatures among locations and (*iii*) The product of the masses at locations $\mathbf{x}$ and $\mathbf{y}$ [54].

In this paper it is shown that, assuming the decaying function in the functional class of power-laws of the distance, the balance principle involves fractional-order non-local residuals. The correspondent temperature equation is obtained in terms of Marchaud-type fractional derivatives in unbounded domains. A different scenario appears as the thermal energy exchange in bounded domains is considered since only the integral contributions to the Marchaud fractional derivatives defined on bounded regions appear. It follows that the divergent algebraic contributions at the borders are not included in the formulation allowing for the position of non-homogeneous Dirichlet boundary conditions straightforwardly. Moreover the Neumann boundary conditions associated to the fractional-order temperature equation involve, only, the gradient of the temperature field as in well-known local heat transport theories.

The effects induced by the non-homogeneous boundary condition is further investigated, in this paper, either for diffusive and ballistic/diffusive thermal energy exchange. The numerical results reported in the analyses describe the temperature field in 1D rigid conductors showing that the proposed model of fractional-order thermal energy exchange may capture the non-uniform temperature distribution observed in Kapitsa experiments as well as in molecular dynamics simulations.

2. The fractional model of thermal energy exchange in rigid bodies: the second law of thermodynamics

In this section the fractional-order model of thermal energy exchange is derived for a diffusive heat transport. In the first part of the section the balance equation as well as the second law of thermodynamics will be shortly recalled. The second part of the section is dedicated to a numerical simulation of the temperature field in a 1D rigid conductor in presence of long-range thermal energy transport. The effects of the differentiation order on the temperature field in bounded conductors have been addressed with a numerical simulation code.

The main idea beyond the proposed model of non-local thermodynamics relies on the assumption that the energy balance at location $\mathbf{x} \in \mathbb{R}^3$ of a rigid body, encapsulated in a subset $V \subset \mathbb{R}^3$ with boundary surface $S = \partial V$, involves the following contributions:

1. The thermal energy flux among adjacent locations, that it is related to the divergence $\mathbf{\nabla} \cdot \mathbf{q}(\mathbf{x},t)$ of the heat flux density vector $\mathbf{q}(\mathbf{x},t)$.
2. A non-local energy transfer, due to the contribution of the elements $\mathbf{y} \in \mathbb{R}^3$ of the body, that it is assumed proportional to the mass densities of the interacting elements at the locations $\mathbf{x}$ and $\mathbf{y}$ as

$$\mathcal{P}^{(nl)}(\mathbf{x},\mathbf{y};t) = \chi^{(nl)}(\mathbf{x},\mathbf{y};t)\rho(\mathbf{x})\rho(\mathbf{y})dV_{\mathbf{x}}dV_{\mathbf{y}} \tag{1}$$

where $\chi^{(nl)}(\mathbf{x},\mathbf{y};t)\rho(\mathbf{y})dV_{\mathbf{y}}$ is the long-range specific energy per unit time transferred at locations $\mathbf{x}$ by the element at the location $\mathbf{y}$ and ρ is the mass density that is time-independent. Under some restriction of the functional dependence of the long-range specific energy $\mathcal{P}^{(nl)}(\mathbf{x},\mathbf{y};t)$, a Marchaud-type, fractional-order, non-local model of thermal energy transport is obtained in *unbounded* domains. In *bounded* domains, instead, only integral parts of fractional-order operators are involved.

This latter consideration yields two key features of the fractional model of long-range heat transport: (*i*) The Non-Homogeneous Dirichlet boundary conditions of the temperature field along the boundary S_d, namely $T(\mathbf{x},t) = \overline{T}(\mathbf{x},t)$ with $\mathbf{x} \in S_d$ may be easily accounted for since the divergent algebraic contribution to the Marchaud fractional derivatives do not appear; (*ii*) The Neumann boundary conditions on the free surface S_n involves, only, the local contribution to the heat transfer in terms of gradients of the temperature field $\nabla \cdot T(\mathbf{x},t)$ with $\mathbf{x} \in S_n$ since the overall residual reads: