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A discrete unified gas kinetic scheme for phonon Boltzmann transport equation accounting for phonon dispersion and polarization

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ABSTRACT

Different from the gray model for phonon transport, the non-gray model takes account of the dispersion and polarization of phonons. Under the consideration of the real dispersion curve, the phonon transport in micro and nanoscale devices is intractable multiscale problem. On the basis of previous work about gray model for phonon transport by a discrete unified gas kinetic scheme (DUGKS), we extend the DUGKS to solving non-gray transport determined by the frequency-dependent phonon Boltzmann equation. The extension is straightforward due to the intrinsic multiscale property of the DUGKS. Four classic test cases, cross-plane heat conduction, in-plane heat conduction, one-dimensional transient thermal grating problem and two-dimensional steady phonon conduction are used to validate our scheme. Numerical results show that the present scheme can accurately capture ballistic-diffusive transport phenomenon in a wide range. This method may provide a powerful numerical tool for a deep research into nanoscale and microscale heat transport.

1. Introduction

It is well known that conventional thermal conduction in solids is governed by the well-established, phenomenological Fourier Law regardless of the details of thermal energy carriers. However, with the rapid development of micro- and nanofabrication and nanotechnology, the characteristic domain size of interest becomes comparable to or smaller than the mean free path of the heat carriers, and the process characteristic time becomes comparable to or smaller than the relaxation time of the heat carriers. In such cases, Fourier's law is confirmed to be invalid for heat transport [1,2]. Phonons, the primary energy carriers in non-metallic solids and most semiconductors, play an important role in theoretical understanding of physical mechanics of thermal transport in these cases. In the last decades, much attention has been paid to the prediction of thermal conductivity of nanostructures composed of silicon, germanium or graphene [3–7]. Interest in the simulation of phonon-mediated heat transport has led to the development of a variety of models, among which kinetic modeling based on the phonon Boltzmann transport equation (pBTE) is widely believed to be the most suitable one accounting for classical size effects. Since microscopic methods (e.g. molecular dynamics, first-principle, lattice dynamics, etc.) are computationally intensive and time-consuming, mesoscopic approaches based on the solution of the pBTE offer a reasonable balance between accuracy and complexity.

However, even so, it is not easy to solve the pBTE in its most rigorous form due to its high dimensionality, intractable collision term and nonlinear phonon dispersion relation. In early studies or even recent studies [3,4,8–11], a single relaxation-time approximation is made and the physics of phonons is neglected, i.e., no dispersion and no polarization is considered. The resulting model is often called gray model. The gray model uses Debye approximation where the relationship between phonon frequencies and wavelengths is linear. The Debye approximation also suggests that the group velocity of phonon is frequency-independent and the material is of isotropy. However, it is well known that phonon dispersion relations are nonlinear for silicon and other low dimension materials. Such an oversimplification may make the gray model inexpensive but not too accurate. Semi-gray model (also called two-fluid model) intends on improving the accuracy of the gray model and keep the low computational requirement [12]. Phonons in semi-gray model are divided into two groups, propagating mode phonons (longitudinal acoustic phonons accounting for transport effects) and reservoir mode phonons (transverse acoustic phonons and optical phonons accounting for capacitative effects). The semi-gray model is less practical because it is a primarily gray model in some sense [13] and two unknown constants (the group velocity and relaxation time) need to be determined. Therefore, it is still

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very necessary to tackle frequency-dependent pBTE to incorporate more physics contained in the nonlinear dispersion relations.

From the point of view of a modeling and simulation, solving spectral pBTE is a non-trivial task. One of the biggest challenges is how to deal with frequency/wave-number of phonons and their interactions. In other words, this problem is a multiscale problem covering a wide range of Knudsen number which is defined as the ratio of the mean free path to the characteristic length. Extensive efforts have been devoted to the multiscale transport in the last two decades. Traditional Monte Carlo method (MCM) and its variants have achieved a great success in phonon transport with the non-linear dispersion curve [14–18]. The advantage of the Monte Carlo method is that it is tractable and almost linearly scalable for large number of dimensions, and is amenable to addressing complex physics via interactions between the stochastic samples. The shortcoming of this method is that it is born with stochastic statistical uncertainty, what's worse, the computational efficiency of the MCM is quite low in or near the diffusive regime due to the time step restriction. Other particle-based and stochastic methods concerning phonon transport include energy-conserving dissipative particle dynamics, a coarse-grained molecular dynamics [19]. As for the efforts in grid-based methods, Minnich and Chen numerically solved the transient one-dimensional frequency-dependent BTE including polarization by using discrete ordinates methods [20]. The finite element analysis is applied to solving ballistic–diffusive phonon heat transport with advancement of computing power [9,21]. In order to improve computational efficiency, hybrid discrete ordinates—spherical harmonics method is designed carefully by Mittal and Mazumder based on the ballistic-diffusive equation. Finite volume solution to the pBTE with mode-dependent phonon properties was developed by Narumanchi et al. [13,22] and their method shows excellent performance in the sub-micron regime. But the calculations of the equilibrium distribution function are not self-consistent. Besides, the convergence issues may make it unsuitable for large domain simulations [23]. Donmezer and Graham [[24] conducted another finite volume simulation and their multiscale model is valid only in diffusive regime and weakly quasi-ballistic regime. Note that most of the finite volume solutions reported in recent years are concerned with the intensity-based Boltzmann transport equation [25–27]. In the present work, we focus on the energy-based form. Different phonon lattice Boltzmann models have been used to simulate various phonon transport phenomena in the recent years [28–34]. In spite of their successes, to the best of the authors' knowledge, there are still several inherent issues more or less such as the coarse temperature in ballistic regime [32,33], and the inconsistencies between isotropic property and the anisotropy lattice speed [31,35].

Discrete unified gas kinetic scheme (DUGKS), proposed by Zhaoli Guo and his collaborators in 2013 [36], is an asymptotic-preserving (AP) scheme and works efficiently and accurately for multiscale problem. The DUGKS is originally designed for kinetic equations based on finite volume method (FVM). The key point for success of DUGKS is the coupled treatment of transport and collision in the flux construction at the cell interface. This is distinguished from many single scale operator splitting methods, where the transport and collision are numerically treated separately. DUGKS has successfully overcome the time step restriction by the collision time. A number of gas flows ranging from subsonic to hypersonic regimes in different Knudsen numbers have been well resolved by this approach [37]. Recently, Zhaoli Guo and Kun Xu [38] employed the DUGKS to solve the pBTE based on discrete ordinate method, and their results show that the DUGKS perform excellently in both diffusive regime and ballistic regime. However, they do not consider the frequency dependence of the distribution function, relaxation time, and group velocity. So the objective of the present work is to develop DUGKS to numerically solve the pBTE considering dispersion and polarization effects.

The rest of the paper is organized as follows. The next section is devoted to the detailed methodology and implementation of the DUGKS for non-gray model. In Section 3, the approach is validated with various numerical tests including cross-plane heat conduction, in-plane heat conduction, one-dimensional transient thermal grating problem and two-dimensional phonon transport problem. Finally, the conclusions are drawn in Section 4.

2. Methodology

2.1. Phonon Boltzmann transport equation

The energy-based Boltzmann transport equation for phonons in the single frequency-dependent relaxation-time approximation is [20,39,40],

$$\frac{\partial g_{\omega,p}(\mathbf{x},\mathbf{s},t)}{\partial t}+v_{\omega,p}\mathbf{s}\cdot\nabla g_{\omega,p}(\mathbf{x},\mathbf{s},t)=\frac{g^{\mathrm{eq}}_{\omega,p}(T)-g_{\omega,p}(\mathbf{x},\mathbf{s},t)}{\tau_{\omega,p}},\tag{1}$$

where $g_{\omega,p}(\mathbf{x},\mathbf{s},t)=\hbar\omega D(\omega,p)[f(\mathbf{x},\omega,p,\mathbf{s},t)-f^{\mathrm{BE}}(\omega,T_{\mathrm{ref}})]$ is the desired deviational distribution function, $g^{\mathrm{eq}}_{\omega,p}(T)$ is the equilibrium deviational distribution function defined below, $v_{\omega,p}$ is the phonon group velocity, and $\tau_{\omega,p}$ is the overall relaxation time due to all scattering processes in combination. Here, $\mathbf{x}$ is the spatial vector, $\mathbf{s}$ is the directional unit vector, t is the time, ω is the phonon radial frequency, T is the local temperature and p refers to phonon polarization or phonon mode. $f(\mathbf{x},\omega,p,\mathbf{s},t)$ is the distribution function of an ensemble of phonons. $f^{\mathrm{BE}}(\omega,T_{\mathrm{ref}})$ is the Bose-Einstein distribution function at the given temperature. The second term in the left hand of Eq. (1) is convective term, the term in the right hand of Eq. (1) result from collision. Assuming that the temperature difference throughout the domain is much less than the reference temperature, $|\Delta T|=|T-T_{\mathrm{ref}}|\ll T_{\mathrm{ref}}$, the equilibrium deviational distribution is proportional to ΔT [20],

$$g^{\mathrm{eq}}_{\omega,p}(T)=\hbar\omega D(\omega,p)[f^{\mathrm{BE}}(\omega,T)-f^{\mathrm{BE}}(\omega,T_{\mathrm{ref}})]\approx C_{\omega,p}\Delta T.\tag{2}$$

where $\hbar$ is Planck's constant divided by 2π, $D(\omega,p)$ is the phonon density of states per unit volume, and $C_{\omega,p}=\hbar\omega D(\omega,p)\frac{\partial f^{BE}}{\partial T}$ is the mode specific heat. The small temperature differences offer acceptable error and significant simplification in linear response regime though it is not indispensable [16]. The small temperature differences also suggest that the properties of phonon is independent of the local temperature, that is, the relaxation time $\tau_{\omega,p}$ and specific heat $C_{\omega,p}$ can be evaluated at the reference temperature T_{ref}. The general law of energy conservation requires the integration of the right hand of Eq. (1) always equal to zero,

$$\sum_p\int_0^{\omega_{\max,p}}\int_{4\pi}\frac{g^{\mathrm{eq}}_{\omega,p}(T)-g_{\omega,p}(\mathbf{x},\mathbf{s},t)}{\tau_{\omega,p}}\mathrm{d}\Omega\mathrm{d}\omega=0,\tag{3}$$

where Ω is the solid angle in spherical coordinates and $\omega_{\max,p}$ is the maximum frequencies corresponding to a given polarization p. Substituting Eq. (2) into Eq. (3) and rearranging Eq. (3), we can obtain

$$\Delta T=\frac{1}{4\pi}\frac{\sum_p\int_0^{\omega_{\max,p}}\int_{4\pi}\frac{g_{\omega,p}(\mathbf{x},\mathbf{s},t)}{\tau_{\omega,p}}\mathrm{d}\Omega\mathrm{d}\omega}{\sum_p\int_0^{\omega_{\max,p}}\frac{C_{\omega,p}}{\tau_{\omega,p}}\mathrm{d}\omega}.\tag{4}$$

Since the deviational distribution function is a function of direction and frequency, the above equations must be solved for all directions and frequencies, and summed over all directions, frequencies, and polarizations. Although this may be more compli-