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Discrete unified gas kinetic scheme for multiscale heat transfer based on the phonon Boltzmann transport equation

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ABSTRACT

Numerical prediction of multiscale heat transfer is a challenging problem due to the wide range of time and length scales involved. In this work a discrete unified gas kinetic scheme (DUGKS) is developed for heat transfer in materials with different acoustic thickness based on the phonon Boltzmann equation. With discrete phonon direction, the Boltzmann equation is discretized with a second-order finite-volume formulation, in which the time-step is fully determined by the Courant–Friedrichs–Lewy (CFL) condition. The scheme has the asymptotic preserving (AP) properties for both diffusive and ballistic regimes, and can present accurate solutions in the whole transition regime as well. The DUGKS is a self-adaptive multiscale method for the capturing of local transport process. Numerical tests for both heat transfers with different Knudsen numbers are presented to validate the current method.

1. Introduction

Many emerging nanostructures involve semiconductors and dielectrics, in which phonon transport is the main mechanism for heat transfer. Heat transfer process in systems with such nanostructures usually involves multiple temporal and spatial scales [1–3], and it is a challenging problem to develop efficient numerical methods that are applicable to different transport regimes. Owing to the breakdown of Fourier law at small time and spatial scales, and the high computational requirement of microscopic molecular dynamics, the phonon Boltzmann transport equation (BTE) [3,4] is regarded to be able to provide a good base for developing numerical methods for multiscale heat transfer when phase coherence effects are unimportant. Actually, many numerical schemes have been proposed to solve the BTE in previous studies [5], including the stochastic Monte-Carlo (MC) method [6–8] and the deterministic discrete ordinates method (DOM) coupled with finite-difference, finite-volume, or finite-element discretization of spatial space [9–13]. The lattice Boltzmann method (LBM), which was originally developed for continuous fluid flows [14], was also applied to phonon transport [15–18].

Generally, the MC method follows a time-splitting algorithm, namely, the dynamics of a simulated particle is decoupled into advection and scattering processes, and thus the time step used is less than the relaxation time, and the grid size is less than the phonon mean-free-path [19]. Consequently, the computational costs of MC method are expensive in the acoustic thick regime, which prohibit its applications for multiscale problems with diffusive region, although it can be quite efficient for ballistic transport. It is also noted that an improved MC method has been developed recently by simulating only the deviation from equilibrium such that the variance can be efficiently reduced in simulating systems with small temperature variations [8]. In the DOM method, the transient and advection terms in the BTE are usually discretized with techniques that are adopted in computational fluid dynamics (CFD), such as upwind (Step) and central (Diamond) finite-difference schemes, or finite-volume schemes with upwind interpolations. These CFD techniques may introduce significant artificial diffusions (low-order schemes) or numerical instability (high-order schemes) [5]. Regarding the LBM for phonon transport, although it has been applied to some nano and multiscale problems [15–18], some studies have shown that LBM may yield unphysical predictions [20].

Recently, a finite-volume discrete unified gas kinetic scheme (DUGKS) for molecule flows ranging from continuum to rarefied regimes has been developed [21,22], which has high accuracy and outstanding robustness. The nice asymptotic preserving (AP) properties also remove the restriction on the time step by the relaxation time that exists in other kinetic methods with direct discretization of the kinetic equation. Furthermore, the finite-volume formulation enables the DUGKS to handle problems with complex

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geometries [23]. Some comparative studies suggest that the DUGKS has better performances over the LBM even for continuum flows [24,25]. In this work, we will extend the DUGKS to phonon transport to construct an efficient method for the whole multiscale heat transport process ranging from diffusive to ballistic regimes.

The remainder of the paper is organized as follows. Section 2 gives a brief introduction of the phonon BTE, and the DUGKS for the BTE is described in Section 3. Some numerical simulations are carried out in Section 4 to test the scheme, and finally a brief summary is given in Section 5.

2. Phonon Boltzmann transport equation

In a rigid crystalline solids, the atomic vibrations from equilibrium positions can be quantized as quasi-particles known as phonons, and the system can be considered as a domain filled with a phonon gas. The angular frequency ω of a phonon is related to the wave number $\boldsymbol{k} \in R^3$ through certain dispersion relations $\omega = \omega_p(\boldsymbol{k})$, with different polarizations or modes of the phonon. The phonon transport can be described by the Boltzmann transport equation in the regime as the wave effects or phase coherence effects are negligible [2],

$$\frac{\partial f_p}{\partial t} + \boldsymbol{v}_p \cdot \nabla f_p = Q_p, \tag{1}$$

where $f_p = f_p(\boldsymbol{x}, \boldsymbol{k}, \boldsymbol{s}, t)$ (or $= f_p(\boldsymbol{x}, \omega, \boldsymbol{s}, t)$) is the distribution function dependent on wave number $\boldsymbol{k}$ (or frequency ω), polarization p, direction $\boldsymbol{s}$, and position $\boldsymbol{x}$ as well as time t; $\boldsymbol{v}_p = \partial\omega/\partial\boldsymbol{k}$ is the group velocity with which the phonon of polarization p travels. The term on the right hand side, Q_p, represents the rate of change of f_p due to scattering interactions. Usually the scattering is very complicated [3], and a more tractable model widely used is the relaxation time approximation,

$$Q_p = -\frac{1}{\tau_p}\left[f_p - f_p^{eq}\right], \tag{2}$$

where τ_p is the relaxation time, f_p^{eq} is the equilibrium distribution of phonons and follows the Bose–Einstein distribution,

$$f_p^{eq} = \frac{1}{\exp\left(\hbar\omega/k_B T\right) - 1}, \tag{3}$$

with $\hbar$ being the Planck's constant divided by 2π and k_B the Boltzmann constant, respectively, and T is the temperature defined later. The effective relaxation time τ_p usually depends on temperature and frequency, and can be estimated using the Matthiessen's rule if the individual scattering processes are independent of each other [1,26],

$$\frac{1}{\tau_p} = \frac{1}{\tau_U} + \frac{1}{\tau_N} + \frac{1}{\tau_b} + \frac{1}{\tau_i} + \cdots, \tag{4}$$

where the relaxation times appearing on the right hand side are those due to the umklapp (U) and normal (N) phonon–phonon scatterings, boundary scattering, impurity scattering, etc. With the effective relaxation time, one can define the Knudsen number of the system, $\mathrm{Kn} = \lambda_0/l_0$, where l_0 is the characterize length of the system, and $\lambda_0 = v_0\tau_0$ is the phonon mean free path with v_0 being a typical value of the phonon group velocity and τ_0 a typical value of the relaxation time.

The total energy and the heat flux can be defined from the phonon distribution function [27],

$$E = \sum_{\boldsymbol{k},p} \hbar\omega(\boldsymbol{k}) f_p(\boldsymbol{k}) = \sum_p \int_{4\pi} \int \hbar\omega f_p(\omega) D_p(\omega) d\omega d\Omega, \tag{5}$$

$$\boldsymbol{q} = \sum_{\boldsymbol{k},p} \hbar\omega(\boldsymbol{k}) \boldsymbol{v}_p(\boldsymbol{k}) f_p(\boldsymbol{k}) = \sum_p \int_{4\pi} \int \hbar\omega \boldsymbol{v}_p f_p(\omega) D_p(\omega) d\omega d\Omega, \tag{6}$$

where $D_p(\omega)$ is the density of state, and Ω is the solid angle. The temperature T of the system can be obtained from $T = E/C_V$, with C_V being the volume specific heat capacity.

Even with the relaxation time approximation, the BTE is still very difficult to be solved due to the high dimensionality. A number of tractable models have emerged to reduce the complex, such as gray model, semi-gray model, non-gray model, and phonon radiative transfer model [1,28]. To illustrate the essence of our numerical method clearly without loss of generality, we will consider the gray model with the Debye's linear dispersion relation in the present work. This simplified model assumes phonons of all polarizations and frequencies are same and the group speed v_g is a constant and the BTE (1) is expressed in terms of the phonon energy density $e''(\boldsymbol{x}, \boldsymbol{s}, t)$ [1],

$$\frac{\partial e''}{\partial t} + \boldsymbol{v} \cdot \nabla e'' = Q \equiv -\frac{1}{\tau}[e'' - e^{eq}], \tag{7}$$

where $\boldsymbol{v} = v_g \boldsymbol{s}$ is the group velocity, τ is the singlet relaxation time, and e'' is the reduced distribution function for energy density,

$$e''(\boldsymbol{x}, \boldsymbol{s}, t) = \sum_p \int \hbar\omega f_p(\omega) D_p(\omega)\, d\omega. \tag{8}$$

Obviously, the total phonon energy E and heat flux $\boldsymbol{q}$ can be determined from e'',

$$E = \int_{4\pi} e''(\boldsymbol{x}, \boldsymbol{s}, t)\, d\Omega, \quad \boldsymbol{q} = \int_{4\pi} \boldsymbol{v} e''(\boldsymbol{x}, \boldsymbol{s}, t)\, d\Omega. \tag{9}$$

The equilibrium distribution function e^{eq} is just the angular average of the total energy,

$$e^{eq}(\boldsymbol{x}, t) = \frac{1}{4\pi}\int_{4\pi} e''(\boldsymbol{x}, \boldsymbol{s}, t)\, d\Omega = \frac{E}{4\pi}. \tag{10}$$

The gray model employs a single phonon group speed v in all directions and a single relaxation time τ independent of polarization and frequency. Despite the simple formulation, the gray model can provide some insightful predictions on the phonon transport behaviors with acceptable accuracy, especially for low-thermal conductivity dielectrics [13,12]. In the diffusive limit ($\mathrm{Kn} \to 0$), it can be shown that the solution of the kinetic Eq. (7) is determined by its average E that obeys the diffusion equation (see Appendix A for details),

$$\frac{\partial E}{\partial t} = \nabla \cdot (\kappa \nabla T), \tag{11}$$

where the thermal conductivity is given by

$$\kappa = \frac{1}{3} C_V v_g^2 \tau. \tag{12}$$

3. Numerical scheme

3.1. Updating rule in finite-volume formulation

Now we present the construction of the discrete unified gas kinetic scheme (DUGKS) for phonon transport based on Eq. (7). First, the continuous solid angle domain Ω is discretized into N discrete angles using the discrete-ordinates method (DOM) based on certain spherical quadratures, and correspondingly we obtain N discrete directions $\boldsymbol{s}_i$. The accuracy of the quadrature employed is required to ensure the exact evaluation of the angular moments of the distribution function up to certain orders, such as