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Hybrid ballistic–diffusive solution to the frequency-dependent phonon Boltzmann Transport Equation

Pareekshith Allu, Sandip Mazumder *

Department of Mechanical and Aerospace Engineering, The Ohio State University, Columbus, OH 43210, USA

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ABSTRACT

The phonon Boltzmann Transport Equation (BTE) is appropriate for modeling heat conduction in semiconductor materials at the nanoscale. However, the BTE is difficult to solve on account of the directional and spectral nature of the phonon intensity, which necessitates angular and spectral discretization, and ultimately results in a large number (typically few hundreds) of four-dimensional partial differential equations. In the ballistic (large Knudsen number) regime, the phonon intensity is highly anisotropic, and therefore, angular resolution is desirable. However, in the diffusive (small Knudsen number) regime, the intensity is fairly isotropic, and hence, angular discretization is wasteful. In such scenarios, the method of spherical harmonics (P_N approximation) may be effectively used to reduce the large number of directional BTEs to a few partial differential equations. Since the Knudsen number is frequency dependent, the decision to preserve or eliminate angular discretization may be made frequency by frequency based on whether the spectral Knudsen number is large or small. In this article, a hybrid method is proposed in which for some frequency intervals (bands), full angular discretization is used, while for others, the P_1 approximation is invoked to reduce the number of directional BTEs. The accuracy and efficiency of the hybrid method is tested by solving several steady state and transient nanoscale heat conduction problems in two and three-dimensional geometries. Silicon is used as the candidate material. It is found that hybridization is effective in significantly improving the efficiency of solution of the BTE—sometimes by a factor of three—without significant penalty on the accuracy.

1. Introduction

Effective thermal management is critical to further miniaturization and improvement of the power density and performance of next-generation electronic and optoelectronic devices. Typical feature sizes (or characteristic length scales) in such devices range between 10 and 1000 nm. In comparison, the dominant carriers of energy in semiconductor materials, namely phonons, have spectral mean free path of the order of a few hundred nanometers. For example, the mean free path of phonons in silicon at room temperature is approximately in the range 10–1000 nm, with the mean around 300 nm [1]. Consequently, heat conduction in such devices cannot be described adequately using continuum equations, namely the Fourier law of heat conduction. The Boltzmann Transport Equation (BTE) for phonons serves as a viable alternative [2,3] for the prediction of non-equilibrium heat conduction in semiconductor materials at the nanoscale.

The BTE for phonons is an integro-differential equation with 7 independent variables: time, 3 spatial coordinates, 2 directional (or angular) coordinates, and frequency. Under the single-time relaxation approximation, the scattering term of the BTE can be significantly reduced (linearized) so that it becomes a 7-dimensional partial differential equation instead of an integro-differential equation. Nonetheless, even the linearized BTE is very challenging to solve because of its high dimensionality. Literature survey reveals that essentially three methods have been employed to date to numerically solve the phonon BTE: (a) the Monte Carlo method, (b) the lattice Boltzmann method, and (c) deterministic discretization-based methods. While the Monte Carlo method is suitable for the inclusion of complex physics such as dispersion, polarization, and various scattering mechanisms, as originally demonstrated by Mazumder and Majumdar [4], and subsequently used by other researchers [5,6], it is expensive for practical engineering applications, especially when high spatial resolution is sought. Recently, variance reduction techniques have enabled use of the Monte Carlo method for solution of the BTE in realistic

* Corresponding author at: Department of Mechanical and Aerospace Engineering, The Ohio State University, Suite E410, Scott Laboratory, 201 West 19th Avenue, Columbus, OH 43210, USA. Tel.: +1 (614) 247 8099; fax: +1 (614) 292 3163.
E-mail address: mazumder.2@osu.edu (S. Mazumder).

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Nomenclature

D	density of states per unit volume [m^{-3}]
f	number density function
f_0	equilibrium number density function
$G_{\omega,p}$	spectral directionally integrated intensity [W m^{-2} rad^{-1} s]
$\hbar$	Dirac (or reduced Planck) constant = 1.0546×10^{-34} [m^2 kg s^{-1}]
$I_{\omega,p}$	spectral directional phonon intensity [W m^{-2} sr^{-1} rad^{-1} s]
$I_{0,\omega,p}$	equilibrium phonon intensity [W m^{-2} sr^{-1} rad^{-1} s]
Kn	Knudsen number, spectral or overall
Kn_c	cutoff Knudsen number
k_B	Boltzmann constant = 1.381×10^{-23} [m^2 kg s^{-2} K^{-1}]
$\hat{\mathbf{n}}$	unit surface normal vector
N_{band}	total number of spectral intervals (or bands)
$N_{\text{band},Kn<Kn_c}$	number of bands for which the Knudsen number is below the cutoff
N_{cell}	number of control volumes (or cells)
N_{dir}	number of control angles (or directions)
p	phonon polarization index
$\mathbf{q}$	heat flux vector [W m^{-2}]
$\mathbf{r}$	position vector [m]
$\hat{\mathbf{s}}$	unit direction vector
t	time [s]
T	absolute temperature [K]
u	internal energy per unit volume [J/m^3]
V_k	volume of cell k [m^3]

Greek

α	degree of specularity
θ	polar angle [radians]
$\boldsymbol{\upsilon}_{\omega,p}$	phonon group velocity vector [m/s]
$\tau_{\omega,p}$	relaxation time scale [s]
ω	angular frequency [rad/s]
Ω	solid angle (sr)
ψ	azimuthal angle [radians]

three-dimensional structures [7]. The lattice Boltzmann method has only been used for the solution of the phonon BTE in simple two-dimensional structures [8,9].

Deterministic solution of the phonon BTE based on discretization in all 7 dimensions has been brought to the limelight by Murthy and co-workers [10–13]. Such solutions make use of the discrete ordinates method and its variant, namely the control angle discrete ordinates method (referred to as the "finite-volume method for radiation" in the radiation literature [14,15]), for angular discretization. The control angle discrete ordinates method (CADOM) has been shown to be superior [14–16] since it mitigates ray effects inherent in the discrete ordinates method. Angular discretization of the 7-dimensional BTE essentially results in a large number of 5-dimensional BTEs since the total solid angle of 4π must be split into smaller solid angles by discretization of the independent polar and azimuthal angles. For example, Mittal and Mazumder [17,18] have shown that approximately 20 angles in each of the polar and azimuthal directions (resulting in a total of 400 solid angles) are necessary to obtain angular grid independent solutions for realistic three-dimensional geometries, particularly when the Knudsen number is large and transport is ballistic in nature. Other studies [19] have employed 64 angles for computations in two-dimensional (2D) geometries. It is the need for angular dis cretization—typically, at least several tens of solid angles—that renders deterministic solution of the BTE computationally challenging. For example, Ali et al. [20] have recently reported solutions to the transient, frequency-dependent phonon BTE in a device-like three-dimensional (3D) geometry discretized using 604,054 tetrahedral control volumes. They reported calculation times of about an hour for a single time-step on a 400-processor parallel machine.

In an effort to improve the computational efficiency for solution of the phonon BTE, several approaches have been explored. The vast majority of these approaches have attempted to utilize the physical attributes of phonon transport to propose a more efficient solution strategy. When the mean free path of a phonon is significantly larger than characteristic size of the system under consideration, its transport is so-called *ballistic*. In such a scenario, the Knudsen number, which is the ratio of the mean free path to the characteristic size of the system, is large, *i.e.*, $Kn \gg 1$. Conversely, when the mean free path of the phonons is small in comparison to the characteristic size of the system, they undergo numerous scattering events, and transport is so-called *diffusive*. In such a scenario, $Kn \ll 1$. In the ballistic regime, transport is highly direction dependent. For example, the energy flux in a given direction (or intensity) may be very large along paths that directly connect hot and cold entities, while it may be small in other directions. Since scattering re-distributes energy directionally, abundant scattering, as is prevalent in the diffusive transport regime, makes the intensity more or less isotropic or direction independent. Based on the preceding discussion, it is fair to conclude that when scattering is rare, it is imperative that the directional nature of the intensity be captured well, while when scattering is dominant, this is not necessary. Consequently, the need for directional discretization of the BTE arises in ballistic regimes, and may be bypassed in diffusive regimes. This fundamental premise has been employed to develop hybrid solution strategies of different flavors for the BTE. One of the earliest hybrid solution strategies to the BTE was proposed by Chen and co-workers [21–23]. They based their method on the so-called Modified Differential Approximation (MDA) [24], originally developed for photon transport. In this approach, the phonon intensity is assumed to be a superposition of a ballistic intensity and a diffusive intensity. The diffusive intensity, by virtue of being isotropic, is determined by invoking the method of spherical harmonics. The resulting model is the so-called ballistic–diffusive equations (BDE) of phonon transport. In the BDE formulation [21–23], Chen and co-workers introduce artificial temperatures, namely "ballistic" and "media" temperatures. These temperatures do not have physical meaning and are introduced as mathematical artifacts. As a result, they make the formulation—in particular, the boundary conditions—difficult to understand and interpret. Also, the surface-to-surface exchange formulation used by Chen and co-workers [21–23] for determination of the ballistic component of the phonon intensity, which employs geometric viewfactors, is prohibitive for complex multi-dimensional geometries, in which case, determination of the viewfactors itself is a monumental task [25]. Mittal and Mazumder [17,18] developed an alternative formulation, also based on the MDA, which eliminates the need to use artificial temperatures. Furthermore, in their approach, the ballistic component of the phonon intensity is determined using the CADOM, making the solution algorithm amenable to large-scale computations in complex geometries. The method has been