Generalized Ballistic-Diffusive Formulation and Hybrid $S_N$-$P_N$ Solution of the Boltzmann Transport Equation for Phonons for Nonequilibrium Heat Conduction

A generalized form of the ballistic-diffusive equations (BDEs) for approximate solution of the Boltzmann Transport equation (BTE) for phonons is formulated. The formulation presented here is new and general in the sense that, unlike previously published formulations of the BDE, it does not require a priori knowledge of the specific heat capacity of the material. Furthermore, it does not introduce artifacts such as media and ballistic temperatures. As a consequence, the boundary conditions have clear physical meaning. In formulating the BDE, the phonon intensity is split into two components: ballistic and diffusive. The ballistic component is traditionally determined using a viewfactor formulation, while the diffusive component is solved by invoking spherical harmonics expansions. Use of the viewfactor approach for the ballistic component is prohibitive for complex large-scale geometries. Instead, in this work, the ballistic equation is solved using two different established methods that are appropriate for use in complex geometries, namely the discrete ordinates method (DOM) and the control angle discrete ordinates method (CADOM). Results of each method for solving the BDE are compared against benchmark Monte Carlo results, as well as solutions of the BTE using standalone DOM and CADOM for two different two-dimensional transient heat conduction problems at various Knudsen numbers. It is found that standalone CADOM (for BTE) and hybrid CADOM-$P_1$ (for BDE) yield the best accuracy. The hybrid CADOM-$P_1$ is found to be the best method in terms of computational efficiency. [DOI: 10.1115/1.4003961]

Keywords: Boltzmann transport equation, ballistic diffusive equation, BTE, BDE, phonon, nonequilibrium heat conduction

1 Introduction

The efficient removal of heat from modern-day solid-state electronic and optoelectronic devices is a daunting task, and overheating is one of the most common causes of device failure. Modeling thermal transport in microscale and nanoscale crystalline materials can provide fundamental understanding of the mechanisms of heat conduction in semiconductor devices.

The mean free path of the energy-carrying acoustic wave packets (or phonons) in silicon at room temperature is approximately 300 nm [1]. On the other hand, characteristic dimensions of modern semiconductor devices range from a few tens of nanometers to a few hundreds of nanometers [2]. Consequently, heat conduction in such devices cannot be described adequately using continuum equations, namely the Fourier law of heat conduction. Nonequilibrium heat conduction has been successfully modeled in the past using the semiclassical Boltzmann transport equation (BTE) for phonons.

Even if the physics of phonons were to be neglected, i.e., no dispersion, no polarization, frequency-independent (or gray), the BTE is a six-dimensional partial differential equation: three spatial coordinates, two angular coordinates, and time. This high dimensionality of the BTE makes it very challenging to solve, even for simple one-dimensional (1D) films. Traditionally, stochastic methods, such as the Monte Carlo method, have found success in solving high-dimensional partial differential equations. For example, the Monte Carlo method has been successfully used to solve the BTE or its variants for rarefied gas (also known as direct simulation Monte Carlo or DSMC) [3], photons (or radiative transport) [4,5], electrons, and other charge carriers [6,7]. 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 prohibitively expensive for practical engineering applications. In the case of phonon transport, for example, studies [8–10] have shown that even simulation of heat conduction in a 1D thin film can require several tens of hours of central processing unit (CPU) time. Perhaps, the most notable disadvantage of using the Monte Carlo method is that the solution inherently contains statistical errors. While these errors can be reduced by using a large number of stochastic samples, they cannot be completely eliminated. Often, the errors are large enough to cause spurious oscillations and nonconvergence if the Monte Carlo solver were to be coupled to a deterministic solver for some other aspect of the problem, such as for charge carrier transport. In light of these issues, it is fair to contend that the Monte Carlo method is useful for generating benchmark solutions for simple problems but not practical for simulating nonequilibrium heat conduction in large-scale devices and deterministic methods for solving the BTE are desired.
Deterministic solution of the BTE for phonons in multidimensional geometry has been attempted and brought to the limelight primarily by Murthy and coworkers [11–13]. The algorithms used by Murthy and coworkers are directly adapted from existing algorithms in neutron and photon (radiation) transport. Most notably, this particular group has used the discrete ordinates method (DOM) on the BTE, averaging and its variants. Over the years, the algorithms have been refined to improve accuracy and efficiency. For example, a switch has been made from the standard DOM to the so-called control angle discrete ordinates method (CADOM) [15,16] to eliminate so-called “ray effects” and “false scattering” [17]. Also, higher-order and more robust discretization schemes in space, such as the SMART scheme [18], has been introduced [11,12] to improve accuracy and convergence. While the discrete ordinates method has shown tremendous promise for solution of the BTE for phonons, it is still quite expensive. In particular, in the ballistic regime (high Knudsen number), a large number of directions (or control angles) have to be used to attain acceptable accuracy, as has been shown in previously published results [11–13], and will also be shown in this article. This implies solution of a large number of partial differential equations. In the diffusive regime (low Knudsen number), on the other hand, when phonon transport is diffusive, use of DOM with high angular resolution is wasteful and, perhaps, use of a simpler diffusive approximation is warranted for improved efficiency. Another method that has often been used to solve the BTE is the method of spherical harmonics (or $P_N$ approximation). In this method, the angular directions are not discretized. Rather, spherical harmonic basis functions, namely Legendre polynomials, are used to capture the angular variations in the intensity analytically. The lowest order spherical harmonics approximation, namely the $P_1$ approximation, reduces the BTE to a single Helmholtz equation with Robin boundary conditions, making it an attractive choice for solution of the BTE since only one partial differential equation has to be solved, as opposed to several tens in the discrete ordinates method. Unfortunately, the $P_1$ approximation is reasonably accurate only in the diffusive (low Knudsen number) regime, and its accuracy at intermediate or high Knudsen numbers is unacceptable, as conclusively demonstrated for photon (radiation) transport [19,20]. Therefore, the $P_1$ approximation is inappropriate for solution of the BTE in truly nonequilibrium scenarios. Higher order $P_N$ approximations, as recently formulated for radiation transport [21], may be used. However, use of higher order $P_N$ approximations is significantly more cumbersome than using the $P_1$ approximation [20,21], and the benefits in terms of improved accuracy is often marginal [20].

The modified differential approximation (MDA) was proposed to remove the shortcomings of the $P_1$ approximation for intermediate and high Knudsen numbers. In this method, first proposed by Olfe [22] and later generalized for radiation transport by Modest [23], the intensity of the energy carrier is split into two components: ballistic and diffusive. The ballistic component is determined using a surface-to-surface exchange formulation that employs geometric viewfactors, while the spherical harmonics approximation is invoked for the diffusive component, for which it is justifiably applicable. The result is a hybrid approach that is expected to be efficient and accurate at all Knudsen numbers. In the past decade, the MDA approach has been adopted for solution of the BTE for phonons by Chen and coworkers [24–26], resulting in the so-called ballistic-diffusive equations (BDEs) of phonon transport. In the BDE formulation proposed by Chen and coworkers [24–26], the specific heat capacity of the material appears as an input. This makes direct comparison with results of the BTE difficult, since the specific heat capacity of the material is not an input in the BTE. Second, Chen and coworkers introduce artificial temperatures, namely ballistic and media temperatures, in their formulation. These temperatures do not have a 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. A final point to note is that the surface-to-surface exchange formulation used by Chen and coworkers [24–26], which employs geometric viewfactors, is prohibitive on two counts: (1) it is very expensive and tedious for complex multidimensional geometries in which case determination of the viewfactors itself is a monumental task [27], and (2) all surfaces in a heat conduction simulations are not necessarily diffuse, and therefore, the use of diffuse geometric viewfactors is limiting in its scope.

In this paper, we present a new hybrid formulation (or BDE formulation) for approximate solution of the BTE. The new formulation does not require a priori knowledge of the specific heat capacity of the material and requires the exact same inputs as the original BTE, making direct comparison with the BTE possible. While the new formulation is based upon the same intensity splitting philosophy originally proposed by Olfe [22] for development of the MDA formulation, the resulting BDEs are solved using procedures that are general enough to be applicable to any arbitrary geometry with arbitrary thermal boundary conditions. The ballistic component is determined, in this case, using the DOM and its variants such as the CADOM, while the diffusive component is determined by invoking the $P_N$ approximation. The result is a hybrid $S_N-P_N$ formulation that is flexible enough to allow any accuracy order. As part of this study, direct comparisons are made with benchmark results obtained by solving the BTE using the Monte Carlo method, as well as standalone DOM or CADOM for two carefully chosen transient heat conduction problems at various Knudsen numbers. While the results shown here are for the gray BTE, the formulation is applicable to the nongray (frequency dependent) BTE without additional modifications.

2 Theory and Mathematical Formulation

Quantized lattice vibrations or phonons are the predominant carriers of thermal energy in semiconductor materials [28]. If the mean free path of the traveling phonons is larger than the characteristic dimension of the device being modeled, thermodynamic equilibrium ceases to exist, and thus, the Fourier law of heat conduction is invalid.

The BTE is a semiclassical equation and has been successfully used to model particles that interact with each other via short range forces and follow a statistical distribution [2,28]. Phonons follow Bose-Einstein statistics and interact with each other via scattering processes, and therefore, can be modeled using the BTE, which may be written as [2]

\[
\frac{\partial f}{\partial t} + v_g \nabla f = \frac{\partial f}{\partial t}_{\text{scattering}}
\]  

where $f$ is the distribution function of an ensemble of phonons and $v_g$ is the group velocity. The left side of Eq. (1) represents change of the distribution function due to motion (or drift), whereas the right-hand-side represents change in the distribution function due to collisions (or scattering). Drift causes the phonon energy distribution function to deviate from equilibrium, while collisions tend to restore equilibrium.

Prior to solution of the BTE for phonons, it is necessary to formulate the right-hand-side of Eq. (1). This scattering term is complicated if all possible scattering mechanisms are considered rigorously. Due to the complexity of the scattering term, simplifications and approximations have to be made to the BTE before it can be solved. The most common approximation used to simplify the BTE is the single relaxation time approximation, whereby the scattering term is expressed as

\[
\frac{\partial f}{\partial t}_{\text{scattering}} = \frac{f_0 - f}{\tau}
\]  

where $f_0$ is the equilibrium number density function (i.e., the Bose-Einstein distribution function) and $\tau$ is the overall scattering time.
time-scale of the phonon due to all scattering processes in combination. For an isotropic wave vector space, the distribution function, \( f_a \), is a function of seven independent variables, i.e., \( f_a(t, \mathbf{r}, \mathbf{s}, \omega) \), where \( t \) is time and \( \omega \) is the angular frequency. The space vector \( \mathbf{r} \) has three components, while the direction vector \( \mathbf{s} \) has two components, namely the polar angle \( \theta \) and the azimuthal angle \( \psi \). The equilibrium Bose-Einstein distribution, \( f_0 \), on the other hand, is independent of direction, i.e., \( f_0 = f_0(t, \mathbf{r}, \omega) \). The group velocity, \( \mathbf{v}_g \), is a function of direction, angular frequency, and temperature, i.e., \( \mathbf{v}_g = \mathbf{v}_g(\mathbf{s}, \omega, T) \), while the scattering time-scale, \( \tau \), is a function of angular frequency and temperature, i.e., \( \tau = \tau(\omega, T) \). Equations (1) and (2) can be combined and written in terms of the phonon intensity as follows [25,29]:

\[
\frac{\partial I}{\partial t} + \mathbf{v}_g \cdot \nabla I = \frac{\partial I}{\partial t} + |\mathbf{v}_g| \nabla \cdot (\mathbf{k}I) = \frac{I_0 - I}{\tau} \tag{3}
\]

where \( \mathbf{v}_g = |\mathbf{v}_g| \mathbf{s} \) and the phonon intensity is defined as [29]

\[
I = I(t, \mathbf{r}, \mathbf{s}, \omega) = |\mathbf{v}_g| \hbar \omega D(\omega)/4\pi \tag{4}
\]

where \( D(\omega) \) is the phonon density of states per unit volume and \( \hbar \) is the Dirac constant.

2.1 Derivation of the BDE. Following the intensity splitting philosophy of Olfe [22], the phonon intensity is next split into two components:

\[
I(t, \mathbf{r}, \mathbf{s}, \omega) = I_b(t, \mathbf{r}, \mathbf{s}, \omega) + I_d(t, \mathbf{r}, \mathbf{s}, \omega) \tag{5}
\]

where \( I_b \) and \( I_d \) are the ballistic and diffusive components, respectively. The ballistic component represents phonons emitted from the boundaries and scattered, while the diffusive component represents phonons that are emitted from within the medium and scattered. The former component is highly directional in nature since phonons, in the absence of scattering, follow a direct line of sight from a hot surface to a cold surface, while the latter component is directionally weak since emission is inherently isotropic whether scattering is present or not. Substitution of Eq. (5) into Eq. (3), followed by separation of the ballistic and diffusive components, yields

**Ballistic:**

\[
\frac{\partial I_b}{\partial t} + |\mathbf{v}_g| \nabla \cdot (I_b \mathbf{s}) = -\frac{I_0}{\tau} \tag{6a}
\]

**Diffusive:**

\[
\frac{\partial I_d}{\partial t} + |\mathbf{v}_g| \nabla \cdot (I_d \mathbf{s}) = \frac{I_0 - I_d}{\tau} \tag{6b}
\]

Since the diffusive intensity field is a directionally weak function, it is justifiable to invoke the first order PN approximation for directional variation in the intensity. Thus, using the PN approximation, the diffusive intensity field may be written as [19,25]

\[
I_d(t, \mathbf{r}, \mathbf{s}, \omega) = J_d(t, \mathbf{r}, \omega) + \mathbf{J}_1(t, \mathbf{r}, \omega) \cdot \mathbf{s} \tag{7}
\]

where \( J_0 \) is a direction independent scalar coefficient, and \( \mathbf{J}_1 \) is a direction independent vector coefficient. The dot product with the direction vector renders the second term in Eq. (7) a scalar. Substitution of Eq. (7) into Eq. (6b) yields

\[
\frac{\partial J_0 + \mathbf{J}_1 \cdot \mathbf{s}}{\partial t} + |\mathbf{v}_g| \nabla \cdot (\mathbf{J}_0 + \mathbf{J}_1 \cdot \mathbf{s} \mathbf{s}) = \frac{I_0 - J_0 + \mathbf{J}_1 \cdot \mathbf{s}}{\tau} \tag{8}
\]

Integrating Eq. (8) over the entire solid angle \( 4\pi \) and noting that \( \int_{4\pi} \mathbf{s} \cdot \mathbf{s} \, d\Omega = 0 \) and \( \int_{4\pi} \mathbf{s} \cdot d\Omega = \frac{4\pi}{3} \delta (\delta \text{ is the identity tensor}) \) [19], we get

\[
\frac{\partial J_0}{\partial t} + |\mathbf{v}_g| \nabla \cdot \left( \frac{1}{3} \frac{\mathbf{J}_1}{\tau} \right) = \frac{I_0 - J_0}{\tau} \tag{9}
\]

Equation (9) has two unknowns, namely \( J_0 \) and \( \mathbf{J}_1 \), and cannot be solved. In order to derive another additional equation to close the system of equations, we multiply Eq. (8) by \( s \) and then integrate the resulting equation over the entire solid angle \( 4\pi \). After tedious algebra, this yields

\[
\frac{\partial \mathbf{J}_1}{\partial t} + |\mathbf{v}_g| \nabla \mathbf{J}_1 = \frac{\mathbf{J}_1}{\tau} \tag{10}
\]

Equations (9) and (10) represent two equations with two unknowns, namely \( J_0 \) and \( \mathbf{J}_1 \). In principle, this equation system is closed and can be solved to determine the two unknowns. Unfortunately, since Eq. (10) is a vector equation, it is quite tedious to solve. In order to eliminate \( \mathbf{J}_1 \) in favor of \( J_0 \), we first differentiate Eq. (9) with respect to time, yielding

\[
\frac{\partial^2 J_0}{\partial t^2} + \frac{1}{3} \frac{\partial J_0}{\partial t} |\nabla \mathbf{J}_1| = \frac{1}{\tau} \left[ \frac{\partial I_0}{\partial t} - \frac{\partial J_0}{\partial t} \right] \tag{11}
\]

Next, we take divergence of Eq. (10) resulting in

\[
\frac{\partial}{\partial t} |\nabla \mathbf{J}_1| + |\mathbf{v}_g| \nabla J_0 = -\frac{\nabla \cdot \mathbf{J}_1}{\tau} \tag{12}
\]

Substitution of Eq. (12) into Eq. (11) yields

\[
\frac{\partial^2 J_0}{\partial t^2} + \frac{1}{3} \frac{\partial J_0}{\partial t} |\nabla \mathbf{J}_1| = \frac{1}{\tau} \left[ \frac{\partial I_0}{\partial t} - \frac{\partial J_0}{\partial t} \right] \tag{13}
\]

Substitution of Eq. (9) into Eq. (13) yields

\[
\frac{\partial^2 J_0}{\partial t^2} + \frac{2}{3} \frac{\partial J_0}{\partial t} |\nabla \mathbf{J}_1| = \frac{1}{\tau} \left[ \frac{\partial I_0}{\partial t} - \frac{\partial J_0}{\partial t} \right] \tag{14}
\]

Equation (14) can be solved to determine \( J_0 \). In principle, once \( J_0 \) has been determined, Eq. (10) can be solved to determine \( \mathbf{J}_1 \), and finally, Eq. (7) provides the diffusive component of the phonon intensity field. However, for heat transfer calculations, we are rarely interested in the intensity. More often, we are interested in determining the heat flux, the integrated (over all solid angles) intensity, and the divergence of the heat flux. Using the PN approximation, the integrated diffusive intensity field may be written as

\[
G_d = \int_{4\pi} I_d \, d\Omega = \int_{4\pi} |\mathbf{J}_0 + \mathbf{J}_1 \cdot \mathbf{s}| \, d\Omega = 4\pi I_0 \tag{15}
\]

since \( \mathbf{J}_1 \) is independent of direction and \( \int_{4\pi} \mathbf{s} \cdot d\Omega = 0 \). Substitution of Eq. (15) into Eq. (14) yields an equation for the directionally integrated diffusive component of the phonon intensity, \( G_d \):

\[
\frac{\partial^2 G_d}{\partial t^2} + \frac{2}{3} \frac{\partial G_d}{\partial t} |\nabla \mathbf{J}_1| = \frac{1}{\tau} \left[ \frac{\partial I_0}{\partial t} - \frac{\partial J_0}{\partial t} \right] \tag{16}
\]

Equation (16) is the governing equation for the diffusive component of the phonon intensity. It is preferable over Eq. (14) since the quantity \( G_d \) has a physical meaning (as discussed above), while \( J_0 \) is simply a mathematical quantity without any physical meaning. We conclude this discussion on derivation of the BDE by noting that the ballistic component of the intensity can be determined by solving Eq. (6a), while the diffusive component can be determined by solving Eq. (16), albeit in integrated form. As to why solution of the integrated intensity (as opposed to the directional intensity) is sufficient for heat transfer calculations will become clear in Sec. 2.2. One final point to note is that solution of both Eq. (6a) and Eq. (16) requires boundary conditions, and the boundary conditions are discussed in Sec. 2.3.
2.2. Heat Flux, Divergence of Heat Flux, and Temperature. The ultimate goal of most heat transfer calculations is to predict the normal heat flux at the boundaries and the temperature distribution inside the medium. The relationship between these engineering quantities and the phonon intensity is discussed in this section.

The heat flux is related to the phonon intensity by the relationship [19]

\[ q = \int q_{\text{sd}} d\Omega \quad (17) \]

which upon application of the intensity splitting philosophy [Eq. (5)], becomes

\[ q = \int q_{\text{sd}} d\Omega = \int (I_b + I_g) q_{\text{sd}} d\Omega = \int I_b q_{\text{sd}} d\Omega + \int I_g q_{\text{sd}} d\Omega = q_b + q_d \quad (18) \]

While the solution of the BTE or the BDE provides a mechanism to determine the heat flux, in order to determine the temperature distribution, one must apply the first law of thermodynamics. For static media, the first law may be written as [30]

\[ \frac{\partial U}{\partial t} = -\nabla \cdot \dot{q} + \dot{q}_{\text{gen}} = -\nabla \cdot \dot{q}_b - \nabla \cdot \dot{q}_d + \dot{q}_{\text{gen}} \quad (19) \]

where \( U \) is the internal energy per unit volume and \( \dot{q}_{\text{gen}} \) is the heat generation rate per unit volume due to other mechanisms, such as electron-phonon or photon-phonon interactions etc. Equation (18) has been made use of to derive the last part of Eq. (19). Invoking the \( P_1 \) approximation to the diffusive component of the heat flux in Eq. (18), we obtain

\[ \dot{q}_d = \int q_{\text{sd}} d\Omega = \int (I_b + I_g) q_{\text{sd}} d\Omega = \frac{4\pi}{3} J_1 \quad (20) \]

Taking divergence of Eq. (20) yields

\[ \nabla \cdot \dot{q}_d = \frac{4\pi}{3} \nabla \cdot J_1 \quad (21) \]

Substitution of Eq. (9) and Eq. (15) into Eq. (21) yields

\[ \nabla \cdot \dot{q}_d = \frac{4\pi}{|v_\|} \frac{I_0}{\tau} - \frac{J_0}{\tau} - \frac{\partial \dot{G}_I}{\partial t} = \frac{1}{|v_\|} \left[ \frac{4\pi I_0}{\tau} - \frac{G_d}{\tau} - \frac{\partial \dot{G}_I}{\partial t} \right] \quad (22) \]

In order to derive an expression for the divergence of the ballistic component of the heat flux, we integrate Eq. (6a) over the all solid angles,

\[ \frac{\partial}{\partial t} \left( \int_{4\pi} I_{\text{bd}} d\Omega \right) + |v_\| \nabla \cdot \left( \int_{4\pi} I_{\text{bd}} d\Omega \right) = -\frac{1}{\tau} \int_{4\pi} I_{\text{bd}} d\Omega \quad (23) \]

Defining an integrated ballistic intensity as \( I_b = \int_{4\pi} I_{\text{bd}} d\Omega \) and using Eq. (18), we get

\[ \frac{\partial \dot{G}_I}{\partial t} + |v_\| \nabla \cdot \dot{q}_d = -\frac{\dot{G}_I}{\tau} \quad (24) \]

Substitution of Eqs. (22) and (24) into Eq. (19) yields

\[ \frac{\partial U}{\partial t} = \frac{1}{|v_\|} \left[ \frac{G_b}{\tau} + \frac{\partial \dot{G}_I}{\partial t} \right] - \frac{1}{|v_\|} \left[ \frac{4\pi I_0}{\tau} - \frac{G_d}{\tau} - \frac{\partial \dot{G}_I}{\partial t} \right] + \dot{q}_{\text{gen}} = -\frac{1}{|v_\|} \left[ \frac{4\pi I_0}{\tau} - \frac{G_d}{\tau} - \frac{\partial \dot{G}_I}{\partial t} \right] + \dot{q}_{\text{gen}} \quad (25) \]

where \( G = G_b + G_d \) is the total integrated (over all solid angles) phonon intensity.

The internal energy of a crystalline material is related to its temperature through the Bose-Einstein distribution and its density of state [2]

\[ U = \sum_p \int_0^{\omega_{\text{max}}} \frac{h_0 D(\omega, p)}{\exp[\hbar \omega/k_BT] - 1} d\omega \quad (26) \]

where the summation is over all polarization branches and \( k_B \) is the Boltzmann constant. If Eq. (26) is substituted into Eq. (25), it becomes clear that determination of the temperature field will require solution of a nonlinear equation. Under the assumption of a linear dispersion relationship and a single polarization branch, we obtain the following relationships

\[ U = 4\sigma_p T^4 \frac{|v_\|}{\pi^2}; I_0 = \sigma_p T^4 \frac{|v_\|}{\pi} \quad (27) \]

where \( \sigma_p = \pi^2 k_B^4 / 40 |v_\|^2 \) is the so-called Stefan-Boltzmann constant for phonons [2]. It is worth noting that the expression for the Stefan-Boltzmann constant includes the group velocity. Only under the assumption of a linear dispersion relationship (or no dispersion) is the group velocity a constant. Consequently, the Stefan-Boltzmann constant for phonons, unlike its photon counterpart, is not a true constant, but one that is applicable only under the assumption of no dispersion.

2.3 Boundary Conditions for the BDE. As discussed in Sec. 2.1, determination of the phonon intensity requires solution to Eqs. (6a) and (16). Equation (6a) is a first-order partial differential equation in space, and therefore, requires only one boundary condition. Physically, the intensity is forward propagating and is required only at the point of emission on the boundary. For submicron heat conduction simulations, two kinds of boundary conditions are relevant. The first kind is where the boundary is a thermalizing boundary, i.e., one that is analogous to a black surface for thermal radiation. It emits phonons based on the equilibrium energy distribution and absorbs any phonons that strike it. Mathematically, this implies

\[ I_0(t, r = r_w, \theta, \omega) = I_0(t, r = r_w, \omega) \quad (28) \]

where \( r_w \) is the location of the boundary (or wall). The second kind is an adiabatic boundary that reflects all phonons striking it and absorbs none. The reflection may be diffuse, specular, or partially specular. Depending on the reflection characteristics of the surface, the total incident radiation to the boundary is redistributed into specific directions. The procedure on how to apply reflection boundary conditions in the context of the DOM or the CADOM, which are the methods employed here, is available elsewhere [11,12] and is omitted here for the sake of brevity.

The boundary conditions for the diffusive component of the phonon intensity are not as straightforward. Since we are solving the governing equation for the integrated intensity, \( G_d \), rather than the intensity itself, the boundary conditions need to be formulated accordingly. The most common procedure to develop boundary conditions for \( G_d \) is to apply Marshak’s procedure [19]. Essentially, this amounts to satisfying flux conservation at the boundaries. The heat flux normal to a boundary is the net effect of phonons emitted from the boundary and the phonons absorbed by the boundary. Thus

\[ q \hat{n} = q_{\text{bd}} \hat{n} + q_{\text{ab}} \hat{n} = \begin{cases} I_0 \hat{n} \hat{s} d\Omega & \text{outgoing} \\ I_0 \hat{n} \hat{s} d\Omega & \text{incoming} \end{cases} \quad (29) \]
where \( \hat{n} \) is the inward facing surface normal to the boundary. If the ballistic component of the heat flux at the boundaries is written as

\[
q_{b} \cdot \hat{n} = \pi J_0 - \int_{\tilde{\omega}_b < 0} I_b \hat{n} \cdot \hat{s} d \Omega
\]  

(30)

it follows from Eqs. (29) and (30) that the diffuse component is

\[
q_{d} \cdot \hat{n} = - \int_{\tilde{\omega}_d > 0} I_d \hat{n} \cdot \hat{s} d \Omega
\]  

(31)

Equation (30) is consistent with the intensity boundary conditions discussed above for the ballistic component. Application of the P1 equilibrium energy distribution, upon rearrangement of Eq. (32), and using Eq. (15), we obtain

\[
q_{b} \cdot \hat{n} = - \frac{\pi J_0 - \frac{2 \pi}{3} J_1 \hat{n}}{\hat{n} \cdot \hat{s} / \Omega}
\]

(32)

Upon rearrangement of Eq. (32), and using Eq. (15), we obtain

\[
q_{d} \cdot \hat{n} = - \frac{\pi J_0}{2} - \frac{G_d}{\tau}
\]

(33)

Substituting Eq. (20) in Eq. (10), we obtain

\[
\frac{\partial q_{d}}{\partial t} + \frac{|v_g|}{2} \frac{4 \pi}{5} J_0 = - \frac{q_{d}}{\tau}
\]

(34)

Performing a dot product of \( \hat{n} \) with Eq. (34), followed by substitution of Eq. (33) and Eq. (15) into the resulting equation yields

\[
\frac{\partial G_d}{\partial t} - \frac{2}{3} |v_g|^2 \hat{n} \nabla G_d = - \frac{G_d}{\tau}
\]

(35)

Equation (35) represents the boundary condition for Eq. (16). It is a boundary condition of the third kind (Robin type) and is applicable to all nonadiabatic boundaries of the computational domain. For adiabatic boundaries or symmetry plains, the net heat flux must be set to zero.

2.4. Solution Algorithm and Numerical Procedure. The preceding sections outline the governing equations that need to be solved and the associated boundary conditions for the BDE. In order to attain the solution to a heat transfer problem using this formulation, the equations need to be solved in a certain sequence, which is described below:

Step 1: Set initial conditions for temperature (internal energy) and the two components of the phonon intensity, namely \( I_0 \) and \( G_d \).

Step 2: Solve for the ballistic component of the phonon intensity, \( I_0 \), using Eq. (6a) subject the boundary condition provided in Eq. (28).

Step 3: Compute the integrated ballistic component of the phonon intensity using \( G_b = \int \sigma_{b} I_0 d \Omega \).

Step 4: Guess the temperature distribution within the whole computational domain. This provides an initial estimate for the equilibrium energy distribution, \( I_0 \), through Eq. (27).

Step 5: Determine the integrated diffusive component of the phonon intensity, \( G_d \), by solving Eq. (16) subject to the boundary condition given by Eq. (35).

Step 6: Solve the overall energy balance equation (Eq. (25)). In conjunction with Eq. (26) or Eq. (27), this provides the new temperature distribution.

Step 7: Repeat steps 5 and 6 until convergence (i.e., temperature stops changing within that particular time-step).

Step 8: Compute heat fluxes at boundaries using Eqs. (30), (33), and (15).

Step 9: Proceed to next time-step and repeat Steps 2–8.

The two most critical and time-consuming steps in the algorithm just described are the determination of the ballistic component of the phonon intensity (step 2) and the diffusive component of the phonon intensity (step 5). As mentioned earlier, the ballistic component is traditionally determined by using a surface-to-surface exchange formulation that makes use of geometric viewfactors between diffuse surfaces, as was done by Chen and co-workers [24–26]. This approach is restrictive because it is difficult to mix diffuse and specular surfaces, as is always prevalent in practical problems. Second, such a method is prohibitively expensive when the geometry is complex (with obstructions and 3D), as has been demonstrated recently for photon transport [27]. In light of these shortcomings of the traditional viewfactor based approach, we chose to use the DOM and the CADOM for the solution of Eq. (6a). CADOM is preferable over DOM for ballistic (high Knudsen number) cases because it alleviates ray effects. The numerical procedures for discretization of the Boltzmann transport equation for phonons using either DOM or CADOM on an unstructured mesh are reported elsewhere [11,31] and are omitted here for the sake of brevity. In this work, both Eqs. (6a) and (16) are discretized on an unstructured mesh of arbitrary topology using the finite-volume procedure. The resulting algebraic equations are solved using the generalized minimum residual (GMRES) solver [32] after incomplete LU (ILU) preconditioning.

An important attribute of the numerical algorithm described above is that only steps 5 and 6 have to be repeated if all boundaries are isothermal. The ballistic equation (directional discrete ordinates equations) is solved only once, i.e., step 2 is executed only once. Change of the medium’s temperature requires repeated solution of only the diffusive component of the phonon intensity (step 5). This implies that in this hybrid method, only a single partial differential equation (Eq. (16)) has to be solved repeatedly within the outer iteration loop that updates temperature of the medium. In contrast, if the DOM or CADOM is used directly for the solution of the BTE, all directional equations in the DOM or CADOM method have to be solved repeatedly. Clearly, this is a notable advantage of the hybrid method (or BDE) over direct solution of the BTE, in terms of computational efficiency. Another advantage of the hybrid approach is that the governing equation for the ballistic component, namely Eq. (6a), is source-less, as indicated by the lack of the \( I_0 \)-containing term. This makes it more amenable to numerical solution in comparison to the original BTE (Eq. (3)), which has this source present.

2.5. Non-Dimensional Form of Equations and Knudsen Number. The degree of nonequilibrium in any nonequilibrium coupled transport-scattering/collision process is dictated by the Knudsen number. In the context of phonon heat conduction, the Knudsen number is defined as the ratio of the mean free path of the energy carrying phonons to the characteristic dimension. If \( L \) is the characteristic length scale of the device being modeled and \( \Lambda \) is the mean free path, then the Knudsen number is defined as

\[
Kn = \frac{\Lambda}{L} \frac{|v_g| \tau}{L}
\]

(36)

Under the gray (frequency independent) assumption, both the scattering time scale, \( \tau \), as well as the group velocity, \( |v_g| \), are constants. Consequently, the Knudsen number is a constant under the gray assumption.

Introducing the nondimensional time and space variables, namely \( x' = x/L; t' = \tau/t \), it is easy to show that Eqs. (6a) and (16) can be rewritten in the following form.
\[
\frac{\partial I_b}{\partial t} + Kn \nabla^* (I_b \delta) = -I_b \tag{37a}
\]
\[
\frac{\partial^2 G_d}{\partial t^2} + 2 \frac{\partial G_d}{\partial t} + G_d - \frac{Kn^2}{3} \nabla^2 G_d = 4\pi I_0 + 4\pi \frac{\partial I_0}{\partial t} \tag{37b}
\]

Equation (37) clearly shows that the Knudsen number is the only parameter that dictates the solution of the governing equations.

In summary, a new set of ballistic-diffusive equations have been developed starting from the Boltzmann Transport equation for phonons. The solution to these equations does not require any inputs other than the boundary conditions, initial conditions, and the Knudsen number. In the following section, two test cases are presented to verify and validate the new formulation by comparing its results with the solutions of the original Boltzmann Transport equation.

3 Results and Discussion

In order to test the new hybrid formulation, two different two-dimensional transient heat conduction problems were considered. The geometry of the first test case was chosen to be a square cavity so that benchmark Monte Carlo results could be generated with relative ease. On the other hand, a more complex irregular geometry was chosen for the second test case in order to demonstrate the generality of the proposed method and numerical algorithms that have been employed to solve the governing equations.

The geometry and boundary conditions of the first test case are shown in Fig. 1. This particular problem is similar to the one considered by Yang et al. [26]. The heater is set to a temperature \(T_H = 200\) K, while the walls are set to a temperature of \(T_C = 100\) K. The overall size of the cavity and the phonon group velocity were fixed, and the scattering time scale was adjusted to vary the Knudsen number. The deterministic calculations were performed using a 160 \times 160 mesh, which was found to be the resolution necessary to obtain grid independent solutions. Each solution was time-marched until steady state was attained. A nondimensional time step of approximately \(10^{-3}\) was used. Within each time-step, six orders of magnitude convergence was enforced. For most cases, this required between five and ten iterations. For DOM, the \(S_8\) approximation (40 angles in 2D) was used, and an equivalent number of control angles were used for CADOM.

For validation of the results, the BTE was also solved using the Monte Carlo method, in addition to the various deterministic methods. For the Monte Carlo simulations, a \(80 \times 80\) mesh was used for collecting spatial statistics. Approximately seven million stochastic samples (phonon bundles) were tracked. Eight ensembles were computed for each case, and the results were post-processed to generate mean values and standard deviations, which are shown as error bars in the subsequent figures. Each Monte Carlo simulation required about 1 day of CPU time, implying that each data point (eight ensembles) required about 8 days of calculation time. Although the initial plan was to perform these computations using a \(160 \times 160\) mesh to be compliant with the deterministic computations, this plan was abandoned later in favor of a \(80 \times 80\) mesh since the finer mesh would have required 32 days of CPU time for each data point.

Figure 2(a) shows the time evolution of the temperature profiles along the centerline of the cavity (from bottom to top) for a Knudsen number of 0.01. The non-dimensional temperature in Fig. 2(a) and all subsequent figures is expressed as \(\left(\frac{T - T_C}{T_H - T_C}\right)\). It is clear from this figure that all methods are fairly accurate for this
acoustically thick (diffusive) case. The solution of the BTE by DOM or CADOM matches exactly with Monte Carlo results, while the solution of the BDE using the hybrid formulation produces slight errors. The corresponding heat fluxes at steady state along the bottom wall are shown in Fig. 2(b). The nondimensional heat flux is expressed as \( q_{\text{wall}} = r_p (T_w^4 - T_c^4) \). Significant differences are observed between the heat fluxes predicted by the Monte Carlo and the heat fluxes predicted by the deterministic methods. However, this may be due to the fact that the Monte Carlo method is not able to resolve the extreme gradients near the intersection of the hot and cold sections of the bottom wall since, for reasons explained earlier, a relatively coarse mesh was used for the Monte Carlo simulations. Only minor differences are observed in the flux predictions between the various deterministic methods. In Fig. 2(b), results of the hybrid viewfactor based BDE, as used traditionally (see Ref. [26]), are also shown, and they appear to match the other deterministic methods, as well.

Centerline temperature distributions for Knudsen number equal to unity (intermediate acoustic thickness) are shown in Fig. 3(a). In this case, the results obtained using the standard discrete ordinates method, either for BTE (DOM-BTE) or BDE (DOM-P₁-BDE), are not very accurate. This is due to the onset of the so-called “ray effect,” as will be discussed in detail shortly. The hybrid method based on CADOM (CADOM-P₁) matches solutions of the BTE obtained using CADOM almost exactly, while both of these results match Monte Carlo results quite well. A slight slip is observed near the walls—an indication of the onset of nonequilibrium transport. The fluxes predicted by the various methods at steady state are depicted in Fig. 3(b). The fluxes predicted by all of the methods appear to be quite accurate.

Results for Knudsen number of 100 (ballistic case) are shown in Fig. 4. The “ray effect” is very pronounced in this case for the standard DOM, as is evident from the oscillations in the temperature profiles, and more so from the heat flux distributions at the top wall. It is also worth noting that for this ballistic case, the overall solution of the hybrid method is dominated entirely by the ballistic component, and thus, the solution of the BTE and the BDE (hybrid method) goes hand in hand and no discernable difference is observed between these two solutions. As evident from Fig. 4(b), the CADOM appears to alleviate the ray effects significantly. For this particular Knudsen number, distinct slips in temperature are observed at the walls, indicative of strongly nonequilibrium transport. The results of the current hybrid approach...
match Monte Carlo solutions of the BTE quite accurately, as long as the CADOM method is used for solution of the ballistic component of the phonon intensity.

The ray effect, exhibited by the standard DOM, is more clearly evident in the steady state temperature distributions shown in Fig. 5. It is clear from Fig. 5(a) that in standard DOM, the energy streaks along discrete directions. The effect is alleviated tremendously by the CADOM method, which integrates the governing equation over solid angles prior to solution of the equations, thereby smoothing out the directional variation in the intensity. Overall, based on the results obtained for this particular test case, it can be concluded that the new BDE formulation produces results that are quite accurate at all Knudsen numbers both for unsteady and steady cases. The results produced by the new BDE formulation, based on the CADOM method for solution of the ballistic component (CADOM-P1), appears to be the most accurate.

The second test case considered is similar to the first test case except that the geometry is not regular, as depicted in Fig. 6. The semicircular section at the bottom may be thought of as a microchannel for cooling. In order to model this irregular geometry, an unstructured mesh, comprised of 9124 triangles was used and is shown in Fig. 6(b). Other than the top heater and the bottom cooling channel, all walls were considered adiabatic and diffuse reflectors, as shown in Fig. 6(a). For this particular case, Monte Carlo simulations were not conducted. Instead, since results of the first test case showed the CADOM method to be quite accurate for solution of the BTE, only this method was exercised for comparison with the hybrid method, i.e., results of CADOM BTE were compared with CADOM-P1 BDE. Higher angular resolution of 80 angles (instead of 40) was used to better capture angular variations in the intensity and to eliminate ray effects.

Figures 7–9 show comparison between the temperature distributions obtained using direct solution of the BTE using CADOM (i.e., CADOM BTE) and that obtained using the hybrid method using CADOM (i.e., CADOM-P1, BDE) for a Knudsen number of unity. The three figures show results for three different instances of time. The results at small times (Fig. 7), predicted by the two methods, are almost identical. At intermediate times (Fig. 8) and at large times (Fig. 9), some differences between the two methods are observed. In particular, the hot front appears to propagate slightly faster in the case of the BTE than in the case of the BDE.
Computational efficiency studies were also performed for the two methods that were considered for the second test case. These efficiency studies were conducted only for steady state cases, i.e., the governing equations were solved iteratively after dropping the time derivatives, rather than time-marching the solution to steady state. For $Kn = 100$, both methods converged in less than ten iterations and required only a few seconds of computational time, while for $Kn = 0.01$, both methods required close to 15,000 iterations and several hours of computational time to attain seven orders of magnitude convergence. Both methods (CADOM BTE and CADOM-P1 BDE) required similar computational times for the second test case. When the adiabatic walls were changed to isothermal walls, for the same test case, the hybrid CADOM-P1 method was found to be at least one order of magnitude faster than the standalone CADOM method for solving the BTE. As discussed earlier, this is due to the fact that in the case of all

![Fig. 7](image1)

**Fig. 7** Comparison of temperature distribution obtained using two different methods for Knudsen number equal to unity and after $t = 0.1$: (a) CADOM BTE and (b) CADOM-P1 BDE

![Fig. 8](image2)

**Fig. 8** Comparison of temperature distribution obtained using two different methods for Knudsen number equal to unity and after $t = 0.1$: (a) CADOM BTE and (b) CADOM-P1 BDE
isothermal walls, it is not necessary to solve the ballistic equation within the outer iteration loop in the hybrid method, thereby making the method considerably more efficient.

4 Summary and Conclusions

A new generalized form of the BDEs for approximate solution of the Boltzmann Transport equation (BTE) for phonons is demonstrated. The derivation of the governing BDE equations, along with appropriate boundary conditions, is presented in full detail. This new formulation, unlike previously published formulations of the BDE [24,25], does not require a priori knowledge of the specific heat capacity of the material. The only input required in this formulation is the phonon scattering time scale (or Knudsen number in nondimensional form), which is the same input required for solution of the original BTE.

In previous instances of solution of nonequilibrium heat conduction problems using the BDE [24–26], the ballistic component of the phonon intensity was determined using a geometric view-factor based surface-to-surface formulation. Such an approach is restrictive for complex geometries and nondiffuse adiabatic surfaces. Another contribution of the current work is that instead of using a view-factor based surface-to-surface formulation, the ballistic component of the phonon intensity is determined by solving the original governing ballistic equation using two different established methods that are appropriate for use in complex geometries, namely the DOM and the CADOM. To demonstrate the new BDE formulation, two two-dimensional transient heat conduction problems are solved, one of which involves an irregular geometry and unstructured mesh. Results of each method for solving the BDE are compared against benchmark Monte Carlo results, as well as solutions of the BTE using standalone DOM and CADOM at various Knudsen numbers. It is found that standalone CADOM (for BTE) and hybrid CADOM-P1 (for BDE) yield the best accuracy. In terms of computational efficiency, the hybrid CADOM-P1 method is found to be comparable or better than the CADOM method for direct solution of the BTE. The standard discrete ordinates method is found to be unacceptable at large Knudsen numbers (ballistic limit) due to “ray effects.”

This article represents the first step toward development of a robust and general method for approximate solution of the Boltzmann transport equation. To the best of the authors’ knowledge, it also represents the first article where various methods for solving the Boltzmann transport equation for phonons, in both its direct and approximate form (e.g., the BDE), are compared directly against Monte Carlo results. Future work will focus on refining the numerical algorithms to attain better computational efficiency and in extending the proposed BDE formulation to incorporate phonon physics, i.e., accounting for dispersion, polarization, and other related nongray effects. Such extensions have already been made and demonstrated [33] to existing BDE formulations [24,25], and therefore, no serious complexities are anticipated with the current formulation.

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Nomenclature

\[ f = \text{number distribution function} \]
\[ f_0 = \text{equilibrium number distribution function} \]
\[ G = \text{integrated (over all directions) total phonon intensity (Wm}^{-2}) \]
\[ G_b = \text{integrated (over all directions) ballistic component of phonon intensity (Wm}^{-2}) \]
\[ G_d = \text{integrated (over all directions) diffusive component of phonon intensity (Wm}^{-2}) \]
\[ h = \text{Dirac constant} = 1.0546 \times 10^{-34} \text{(m}^2\text{kg.s}^{-1}) \]
\[ I = \text{total phonon intensity (Wm}^{-2}\text{sr}^{-1}) \]
\( I_0 \) = equilibrium phonon intensity (Wm\(^{-2}\)sr\(^{-1}\))
\( I_b \) = ballistic component of phonon intensity (Wm\(^{-2}\)sr\(^{-1}\))
\( I_d \) = diffusive component of phonon intensity (Wm\(^{-2}\)sr\(^{-1}\))
\( J_0, J_1 \) = constants in spherical harmonics expansion (Eq. (7))
\( k_B \) = Boltzmann constant = \( 1.381 \times 10^{-23} \) (m\(^2\)kg.s\(^{-2}\)K\(^{-1}\))
\( K_n \) = Knudsen number
\( L \) = characteristic length scale (m)
\( n \) = inward pointing unit surface normal vector
\( p \) = phonon polarization
\( q \) = total heat flux (Wm\(^{-2}\))
\( q_b \) = ballistic component of heat flux (Wm\(^{-2}\))
\( q_d \) = diffusive component of heat flux (Wm\(^{-2}\))
\( s \) = unit direction vector
\( t \) = time (s)
\( t' \) = nondimensional time
\( T \) = thermodynamic temperature (K)

### Greek Symbols

\( \psi \) = phonon group velocity vector (m/s)
\( \tau \) = overall scattering time scale (s)
\( \omega \) = angular frequency (rad/s)
\( \Omega \) = solid angle (sr)
\( \sigma_0 \) = Stefan-Boltzmann constant for phonons (Wm\(^{-2}\)K\(^{-4}\))

### References


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