The lattice Boltzmann Peierls Callaway equation for mesoscopic thermal transport modeling

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The lattice Boltzmann Peierls Callaway (LBPC) method is a recent development of the versatile lattice Boltzmann formalism aimed at a numerical experiment on mesoscopic thermal transport in a multiphase phonon gas. Two aspects of mesoscopic thermal transport are discussed: the finite phonon mean free path and the interface thermal resistance. Based on the phonon momentum screening length measured in the LBPC computational apparatus, the validity of the Umklapp collision relaxation time in the Callaway collision operator is examined quantitatively. The discrete nature of the spatio-temporal domain in the LBPC method, along with the linear approximation of the exponential screening mechanism in the Callaway operator, reveals a large discrepancy between the effective phonon mean free path and the analytic phonon mean free path when the relaxation time is small. The link bounce back interface phonon collision rule is used to realize the interface thermal resistance between phonon gases with dissimilar dispersion relations. Consistent with the Callaway collision operator for the bulk phonon dynamics, the interface phonon collision process is regarded as a linear relaxation mechanism toward the local pseudo-equilibrium phonon distribution uniquely defined by the energy conservation principle. The interface thermal resistance is linearly proportional to the relaxation time of the proposed phonon interface collision rule.

\textbf{Keywords:} lattice Boltzmann method; link bounce back collision rule; Boltzmann Peierls equation; phonon hydrodynamics; Kapitza length; interfacial thermal resistance

1. Introduction

Throughout the last decade, thermal management in electronic devices has been attracting growing attention. The increasing thermal load in miniaturizing micro/nanoscale electronic devices needs to be quickly dissipated for the performance and the mechanical stability of the device not to be hampered; this constitutes a challenge for the further scale-down of the characteristic size of the device. Possible solutions lie in the combination of novel cooling strategies and the use of novel materials with a higher thermal conductance.
A reliable and efficient numerical modeling scheme for heat transport at the device scale will complement the experimental efforts for effective thermal control.

Traditional thermal modeling of a heterogeneous solid medium at macroscales constitutes a well-defined boundary value diffusion problem. The geometric location of boundaries between different materials, along with the well-defined thermal diffusivity and the heat capacity of each material, determines the effective thermal properties of the system. However, as the characteristic size of the system decreases, two distinct features gradually emerge in terms of heat transfer. One regards the resistance of the system to the energy flux. The effective resistance to the flux comes from both the bulk materials and the interface between them. At the macroscale, the surface resistance is, though finite, normally neglected compared to the magnitude of the bulk resistance. However, the enhanced surface-to-volume ratio in small-scale devices allots a high portion of the effective resistance to the surface, solely due to the decrease in the bulk resistance. Another feature regards the very definition of the thermal conductivity, i.e. the product of the thermal diffusivity and the heat capacity. As the characteristic system size approaches the mean free path of the energy carrier, the material properties become dependent upon the size and the boundary conditions. Without a well-defined heat conductivity as a material property, the traditional heat transfer model based on the Fourier law becomes obsolete. Although microscopic modeling, without any assumption about the finite volume of the continuum material point, holds the principle validity in the small scale modeling, the practice often finds interest in the device scale at which the computation involving microscopic atomic degrees of freedom becomes too expensive and of superfluous information. Therefore a resolution is sought after in the mesoscale where the microscopic information is properly coarse-grained. In a solid device, the fundamental thermal energy carriers are electrons and phonons, on which the coarse-graining, therefore, should be executed. In this article, our interest, henceforth, is on the heat transfer mediated by the phonon dynamics.

The Boltzmann Peierls (BP) equation for phonon transport has long been utilized in studies of the phonon gas, including the second-sound mode, the phonon viscosity and the phonon hydrodynamics [1–6]. The BP equation has been favored as the model of choice for the heat transfer mediated by phonon dynamics at the mesoscale due to its straightforward coarse-graining procedure connecting the microscopic phonon distribution function with the macroscopic thermal observables as the moments of the distribution function [7–14].

The lattice Boltzmann (LB) method is an efficient route to solving the general Boltzmann kinetic equation, especially noted for its exceptional numerical efficiency due to the local nature of its microdynamics leading to superb parallel computing opportunities. The LB method has been developed for various transport problems including magnetohydrodynamics, plasma dynamics, multiphase flow, and so forth [15–17]. In the LB scheme, the coordinate space and the momentum space are coherently discretized by a single lattice structure, which is inherited from the lattice gas cellular automata [18]. Moreover, the momentum set is of maximal discretization, retaining the minimal symmetry property required to recover the desired macroscopic transport equation [19]. In a sense, the LB scheme uses the minimal phase space to recover the macrodynamics sought after.

Guyer was the first to recognize the efficiency of the LB scheme and adapted it directly to the BP equation in studying the second-sound mode in a homogeneous phonon gas [21]. Although the general form of the Boltzmann kinetic equation can model transport phenomena in a broad range of spatio-temporal scales, it is the approximation used in the collision operator that determines the level of coarse-graining adopted in the specific model. Guyer tested both the deterministic three-phonon collision operator and the mesoscopic Callaway phonon collision operator. For efficient notation, we shall call the
LB scheme of the BP equation with the Callaway collision operator the lattice Boltzmann Peierls Callaway (LBPC) equation from now on. Jiaung and Ho revisited Guyer’s work and showed, through multiscale Chapman–Enskog analysis on the D2Q9, i.e. the two-dimension, nine-velocity LBPC model that the macrodynamics of the LBPC equation is a phonon thermal wave equation (PTWE) with an additional fourth-order spatial derivative term to the dual phase lag thermal wave equation [22].

As mentioned at the beginning, the important factors that must be included in the mesoscale thermal modeling are the interface thermal resistance and the finite phonon mean free path. So far, applications of the LBPC equation have concerned the effect of the phonon mean free path or the complex device geometry on the heat transfer in a phonon gas with a spatially homogeneous dispersion relation and heat capacity [22, 23]. Recently, adopting the link bounce back collision rule for the velocity boundary condition on the moving fluid–solid interface proposed by Ladd [24], Lee et al. reported a phonon-interface collision scheme in the LBPC equation to model the interface thermal resistance. Their approach followed two physical guidelines [25]: First, the phonon-interface collision is an Umklapp process conserving the total energy only [26]. Secondly, all phonon collision processes throughout the system are treated at the same level of coarse-graining in the spirit of Callaway collision operators [27]. The phonon-interface collision process is regarded as a mechanism for reaching the local pseudo-equilibrium phonon distribution, toward which a linear relaxation is approximated. Just as the relaxation time for the bulk phonon collision process determines the mean free path of the phonon dynamics in the bulk, the relaxation time for the phonon-interface collision process determines the Kapitza length of the thermal interface [28]. Lee et al. extended the LBPC equation to a multiphase phonon gas where phonon phases with different heat capacities coexist.

In this article, we review the recent developments of the LBPC model for a multiphase phonon gas. In particular, we focus on how the LBPC model incorporates two aspects characterizing mesoscale thermal transport; the size-dependent thermal conductivity due to the finite phonon mean free path and the interface thermal resistance based on a mesoscopic ansatz on the phonon-interface collision process.

2. Theory and method

The Boltzmann Peierls equation for phonon transport with a Callaway collision operator, i.e. the BPC equation,

$$\left( \partial_t + v_{g,k} \cdot \nabla_r \right) f^\sigma(t, \mathbf{r}, \mathbf{k}) = \frac{f_{N}^{\sigma,eq} - f^\sigma}{\tau_N} + \frac{f_{U}^{\sigma,eq} - f^\sigma}{\tau_U},$$

(1)

describes the time evolution of the single-phonon distribution function, $f$, in the six-dimensional phase space $(\mathbf{r}, \mathbf{k})$ of physical coordinates and momenta. $v_{g,k}^\sigma$ is the group velocity of a phonon with polarization $\sigma$ and momentum $\hbar \mathbf{k}$, where $\hbar$ is the reduced Planck constant. The phonon collision operator on the right-hand side of Equation (1) is proposed by Callaway as a revision of the Bhatnagar–Gross–Krook operator [27, 29]. The mesoscopic nature of the BPC equation is set by the description of the collision process. In the BPC equation, the phonon collision process is approximated as a mechanism involving a collection of collisions to restore the local equilibrium phonon distributions. $\tau_U$ and $\tau_N$ are the characteristic collision times for the linear relaxation of $f^\sigma$ toward the local equilibria. The Callaway operator considers two types of phonon collision processes. One is the energy-conserving but momentum-destroying Umklapp process, through which the phonon distribution reaches the Planck distribution,
defined by the local temperature, $\beta = 1/k_B T$, where $k_B$ is the Boltzmann constant and $\hbar \omega$ is the phonon energy, where $\omega$ is the angular frequency. The other process is the normal collision process conserving both the total energy and the total crystal momentum, through which the phonon distribution restores the displaced Planck distribution,

$$f_{\sigma,eq}^U[\beta(t, r)] = \frac{1}{e^{\beta \hbar \omega} - 1},$$

where $\hbar \omega$ is the phonon energy, where $\omega$ is the angular frequency. The other process is the normal

$$f_{\sigma,eq}^N[\beta_d(t, r), u(t, r)] = \frac{1}{e^{\beta_d (\hbar \omega - \hbar k \cdot u)} - 1},$$

Further discussion is necessary regarding the Callaway collision operator which sets the BPC equation apart from rather traditional modeling approaches at scales other than mesoscale. As briefly stated above, the spatio-temporal scale of a specific model is set by the approximation in the collision process. If the collision process is treated as a deterministic event involving a finite number of phonons, then the spatio-temporal scale of the model becomes microscopic. Modeling strategies involving atomic degrees of freedom, such as molecular dynamics simulations and the Boltzmann Peierls equation with three-body phonon collision dynamics, belong to this category. Local equilibrium is easily accessible with microscopic simulations. However, transport phenomena due to gradients in the local equilibrium are computationally often too expensive for microscopic simulations. On the other hand, at the macroscopic spatio-temporal scale, the carrier distribution is assumed to be at local equilibrium all the time. Fourier’s law of heat conduction belongs to this category. The spatio-temporal scale of the BPC equation is tuned to model the process between these two limits.

Macroscopic observables such as the temperature field and the heat flux field are moments of the distribution function $f$. Hypothetically, if the phonon collision in the bulk is dominated by the normal process, then the time evolution of the temperature field, $\beta_d(r, t)$, follows that of the wave equation. On the other hand, when the phonon collision is dominated by an Umklapp process, the temperature field, $\beta(r, t)$, shows diffusion dynamics. The macrodynamics of the BPC equation can be roughly stated as a drift-diffusion equation for the temperature field. The precise macrodynamics of the BPC equation is a phonon thermal wave equation (PTWE) with an additional fourth-order spatial derivative term to the dual phase lag thermal wave equation [22].

The lattice Boltzmann Peierls–Callaway (LBPC) equation follows when Equation (1) is expressed on the discrete phase space of an LB model:

$$\frac{n^\sigma_i (r + \frac{v_i}{2} \epsilon, t + \Delta t + \Delta t) - n^\sigma_i (r, t)}{\Delta t} = \frac{n_{i,N}^{\sigma,eq}(r, t) - n^\sigma_i (r, t)}{\tau_N} + \frac{n_{i,U}^{\sigma,eq}(r, t) - n^\sigma_i (r, t)}{\tau_U}. $$

(4)
Here, \( n_i^r(\mathbf{r}, t) \) is the number distribution function of phonons with polarization \( \sigma \) in the direction of \( \mathbf{c}_i \) at position \( \mathbf{r} \) and time \( t \). \( \mathbf{c}_i \) is the velocity vector connecting the lattice node at \( \mathbf{r} \) with the neighboring node at \( \mathbf{r} + \mathbf{c}_i \Delta t \). \( c \) is the unit speed of the LB model, and \( c = \Delta x/\Delta t \), where \( \Delta x \) is the lattice spacing and \( \Delta t \) is the discrete time step to update the distribution function. As discussed later in this section, \( n_{i,N}^{\sigma,eq} \) and \( n_{i,U}^{\sigma,eq} \) are the displaced Planck distribution and the Planck distribution, respectively, toward which \( n_i^r \) linearly relaxes with relaxation times of \( \tau_N \) and \( \tau_U \). We use the D3Q19, i.e., three-dimensional, 19-velocity LB model in this study. However, because the theory is presented in a general manner independent of the specific LB model, the details of the D3Q19 model itself that are unrelated to the phonon dynamics can be found in the popular references [19, 20].

The velocity space is discretized with a set of finite velocities \( \mathbf{c}_i \) linking the lattice nodes. For example, the nodes of the hypercubic lattice of the D3Q19 LB model are connected by 19 link vectors \((i = 0, 1, \ldots, 18)\): six links connecting the nearest neighbors, 12 links connecting the second nearest neighbors, and a link connecting the node to itself. Depending on the link direction \( i \) and the polarization \( \sigma \), a phonon has momentum \( \mathbf{p}_i^r = p\mathbf{c}_i \), group velocity \( \mathbf{v}_g^\sigma = \mathbf{v}_g^0 \mathbf{c}_i \), and energy \( \epsilon^\sigma = \mathbf{p}_i^r \cdot \mathbf{v}_g^\sigma = p\mathbf{v}_g^\sigma \mathbf{c}_i \cdot \mathbf{c}_i = \epsilon^\sigma \mathbf{c}_i \cdot \mathbf{c}_i \), where \( p, \mathbf{v}_g^\sigma \), and \( \epsilon^\sigma \) are parameters converting lattice units to physical units. Therefore, the phonon dispersion relation of the LBPC model is given by \( \epsilon^\sigma = p\mathbf{v}_g^\sigma \). Multiple polarizations can be modeled by assigning a different dispersion relation per polarization. Here, we simplify this model by assuming single polarization, whose group velocity coincides with the LB unit speed, \( \mathbf{v}_g^\sigma = \mathbf{v}_g = c \). An extended formalism involving multiple polarizations is straightforward and can be found elsewhere [25].

The LB dynamics is composed of the collision step and the propagation step. Equation (4), simplified for single polarization, can be written as follows to explicitly show the two steps,

\[
n_i \left( \mathbf{r} + \mathbf{c}_i \frac{\mathbf{v}_g}{c} \Delta t, t + \Delta t \right) = n_i^r(\mathbf{r}, t) = (1 - \lambda_N - \lambda_U)n_i(\mathbf{r}, t) + \lambda_N n_{i,N}^{eq} + \lambda_U n_{i,U}^{eq},
\]

where \( \lambda_{N[U]} = \Delta t/\tau_{N[U]} \) are mixing parameters. The post-collision distribution, \( n_i^r \), is a mixture of the pre-collision distribution, \( n_i \), and the local equilibrium distributions, \( n_{i,N}^{eq} \) and \( n_{i,U}^{eq} \). The propagation step carries \( n_i^r \) from the lattice node at \( \mathbf{r} \) to the node at \( \mathbf{r} + \mathbf{c}_i \Delta t \) in time \( \Delta t \). If the over-damping of \( n_i \) is to be avoided, \((1 - \lambda_N - \lambda_U)\) must not be negative. Nevertheless, in practice, it is recommended to keep \((1 - \lambda_N - \lambda_U)\) close to zero for two reasons. First, as the fraction of the non-equilibrium distribution, \( n_i \), increases in the post-collision distribution, the underlying lattice feature starts to emerge in the macroscopic observables of the temperature and heat flux, leading to anisotropic heat wave propagation from a point heat source. As \( \lambda_U \) determines the phonon mean free path, \( \lambda_N \) needs to be close to \( 1 - \lambda_U \) to erase the artifact due to the underlying lattice structure. The second reason, which is minor, is that, because the definition of temperature assumes local equilibrium, a large fraction of the non-equilibrium distribution makes the spatio-temporal resolution of temperature measurement coarser.

The local equilibrium distribution in the LB model is given by a linear expansion of the global equilibrium distribution subject to the local disturbances of the macroscopic collision invariants [19]. At an ambient temperature of \( T_0 \) and a drift velocity \( \mathbf{u}_0 = 0 \), a strict global thermal equilibrium establishes the Planck distribution on all lattice sites: \( w_i/(e^{\beta_0 \epsilon_i} - 1) \), where \( \beta_0 = 1/k_B T_0 \) and \( w_i \) is the weight factor depending on the specific LB model [19]. If a local node at \( (\mathbf{r}, t) \) is subject to the perturbations of the temperature \( \theta(\mathbf{r}, t) = (T(\mathbf{r}, t) - T_0)/T_0 \) and the phonon drift velocity \( \mathbf{u}(\mathbf{r}, t) = (\mathbf{u}(\mathbf{r}, t) - \mathbf{u}_0)/\mathbf{v}_g \) from
$T_0$ and $u_0$, then the local equilibrium distributions at $(r, t)$ can be approximated to first order in the linear expansion of the global equilibrium as

$$n_{i,U}^\text{eq} = w_i (A_i - \beta_0 \epsilon_i B_i \theta),$$

and

$$n_{i,N}^\text{eq} = w_i (A_i - \beta_0 \epsilon_i B_i \theta - \beta_0 \epsilon_i \boldsymbol{c}_i \cdot \tilde{\boldsymbol{u}}),$$

where $A_i = 1/(e^{\beta_0 \epsilon_i} - 1)$, $B_i = \partial A_i / \partial (\beta_0 \epsilon_i) = -A_i (1 + A_i)$, and $\epsilon = p v_g$. Those two temperatures of Equations (2) and (3) become one identical temperature in Equations (7) and (6), because $\sum_i \epsilon_i \boldsymbol{c}_i \cdot \tilde{\boldsymbol{u}} = 0$ up to first-order perturbation of the global equilibrium distribution.

The calculations of $\theta(r, t)$ and $\tilde{\boldsymbol{u}}(r, t)$ must proceed the collision step to determine $n_{i,U}^\text{eq}$ and $n_{i,N}^\text{eq}$, for which the conservation laws for the local collision invariants are utilized. The macroscopic energy, $E$, and the momentum, $P$, are moments of $n_i$, and also collision invariants of the Umklapp and the normal processes, respectively. With Equation (6), the energy conservation of the Umklapp process,

$$E(t, r) = \sum_i \epsilon_i n_i(r, t) = \sum_i \epsilon_i n_{i,U}^\text{eq}(r, t),$$

has $\theta(r, t)$ as the only unknown. Once $\theta(r, t)$ is determined from Equation (8), the conservation of momentum of the normal collision process with Equation (7) determines the local drift velocity $\tilde{\boldsymbol{u}}(r, t)$:

$$P(t, r) = \sum_i p_i n_i(r, t) = \sum_i p_i n_{i,N}^\text{eq}(r, t).$$

Other macro-observables can be calculated as higher moments of $n_i(r, t)$. The heat flux vector, $Q(r, t)$, which is not a collision invariant, turns out to be the sum of the pre-collision heat flux, $Q^\text{pre} = \sum_i v_i \epsilon_i n_i$, and the post-collision heat flux, $Q^\star = \sum_i v_i \epsilon_i n_i^\star$:

$$Q(t, r) = \sum_i v_i \epsilon_i \left[ n_i(r, t) + n_i^\star(r, t) \right]$$

$$= \sum_i v_g \epsilon \boldsymbol{c}_i \cdot \boldsymbol{c}_i \left[ n_i(r, t) + n_i^\star(r, t) \right].$$

Because of the isotropy of the Planck distribution, $Q^\star$, diminishes completely when the phonon collision is dominated by the Umklapp process; $\lambda_U = 1$ and $\lambda_N = 0$. However, $Q^\star$ is finite when $\lambda_U < 1$, and becomes of comparable magnitude to $Q^\text{pre}$ when the Umklapp collision is sparse: $\lambda_U \simeq 0$. In a single-phase phonon gas with a homogeneous dispersion relation with regions of different phonon mean free paths, it is the combined heat flux $Q(r, t)$ that matches across the regional boundaries.

To simulate phonon scattering at the interface between two materials with different phononic properties, the LBPC model is modified to incorporate the link bounce back collision scheme which is based on a local rule applied to the distribution functions [24]. For the phonon collisions, the local rule is a direct energy exchange between phonon
populations at the interface. The interface is constructed by placing a boundary node in the middle of every link connecting the lattice nodes of two different materials. Figure 1 shows an example, where an arbitrarily shaped interface is approximated by a collection of boundary nodes. Boundary nodes break those links connecting different materials in the middle, and phonons moving along the link would collide with the boundary node and be bounced back to the lattice node it came from. The link bounce back collision rule shows the second-order accuracy for planar surfaces and was thoroughly studied and compared with other types of boundary collision rules [30]. The advantages of the link bounce back collision rule to other schemes are in its straightforward implementation and the numerical efficiency which does not hamper the local nature of the LB dynamics.

When there is a boundary node in the middle of the link connecting the node at $r$ and the node at $r + c_i \Delta t$ as shown in Figure 2(a), the phonons of $n_i(r, t)$, incident on the boundary node, experience a boundary collision, and reflect back to the original position with the distribution of $n_j(r, t + \Delta t)$ as shown in Figure 2(c). Notice the change in the direction of the phonon momentum from $c_i$ to $c_j$ due to reflection at the boundary: $c_j = -c_i$. If a complete reflection happens at the boundary so that $n_j(r, t + \Delta t) = n_i(r, t)$, the interface would be of perfect thermal insulation with an infinite thermal resistance ($\rho = \infty$).

In the LBPC model discussed in the previous subsection, the Callaway collision operator regards the phonon–phonon collision process as a mechanism to reach the corresponding local equilibrium distribution, disregarding the microscopic rigor of the collision [27]. In terms of the thermal interface between phonon gases, a microscopic description of the phonon interface collision involves the energy transmission coefficient of each phonon microstate [31–33]. In the mesoscopic spatio-temporal scale, set by the Callaway
collision operator, however, a collection of microscopic collisions, rather than an individual collision, is regarded as approximating the linear nature of the relaxation toward local equilibrium. Applying the same level of coarse-graining to all local phonon collision processes, both in the bulk and on the interface, the ansatz of the interface collision rule follows:

\[
\frac{n_j(r, t + \Delta t) - n_i(r, t)}{\Delta t} = \frac{n_{j, U}^{\text{peq}}(r_b, t) - n_j(r, t)}{\tau_I}, \tag{11}
\]

where \( r_b = r + c_i \Delta t/2 \). The boundary collision is regarded as a relaxation process toward the pseudo-equilibrium distribution, \( n_{j, U}^{\text{peq}}(r_b) \), with a linear relaxation time parameter \( \tau_I \).

The distribution \( n_{j, U}^{\text{peq}}(r_b) \) is called a pseudo-equilibrium, because the collision happens at the interface where true thermodynamic equilibrium is not well defined. The \( U \) in the subscripts of \( n_{j, U}^{\text{peq}} \) indicates that the phonon collision at the interface is an Umklapp process where the total momentum is not a collision invariant [26]. The interface collision occurs only when the propagating phonon distribution encounters the boundary node on the link. Equation (11) is also a mixing scheme, and can be rephrased to explicitly show that:

\[
n_j(r, t + \Delta t) = n_j^*(r + c_i \Delta t, t) = (1 - \lambda_I) n_j(r, t) + \lambda_I n_{j, U}^{\text{peq}}(r_b, t), \tag{12}
\]

where \( \lambda_I = \Delta t/\tau_I \). As illustrated in Figure 2(b), by placing the mixed distribution after collision on the opposite end of the link, the population bounces back to the original node facing away from the boundary node after \( \Delta t \). Because the boundary node is placed at the middle of the link, \( \tau_I \) is equal to or greater than \( 0.5 \Delta t \), which gives \( 0 \leq \lambda_I \leq 2 \). When the mixing parameter \( \lambda_I \) is zero, then \( n_j(r, t + \Delta t) = n_j(r, t) \), which recovers the interface with an infinite thermal resistance (\( \rho = \infty \)) discussed above. The other limiting case of a thermal interface is that of zero thermal resistance (\( \rho = 0 \)) when \( \tau_I = 0.5 \Delta t \).
It turns out that the pseudo-equilibrium distribution on the boundary node is uniquely determined by the collision invariant. Because the boundary collision is an Umklapp process, the ansatz of the pseudo-equilibrium distribution follows the Planck distribution of Equation (6),

\[ n_{j,U}^{\text{peq}}(r_b, t) = w_j \left\{ A_j - \beta_0 \epsilon_j B_j \theta^{\text{eff}}(r_b, t) \right\}, \] (13)

where \( \theta^{\text{eff}} \) is the effective temperature at the boundary node. It is called “effective” because the boundary temperature is not a thermodynamic property. Here, \( \theta^{\text{eff}} \) is present rather as a numerical variable to satisfy the energy conservation principle. When the phonon distributions of two different materials encounter each other at the boundary node, as shown in Figure 2, the total energy of the incoming populations before the collision is \( \epsilon_j n_j(r, t) + \tilde{\epsilon}_j \tilde{n}_j(r + c_i \Delta t, t) \), where a tilde above the variable is used to distinguish the variables belonging to different phonon phases. Assuming complete relaxation toward the pseudo-equilibrium, the total energy of the outgoing population is \( \epsilon_j n_{j,U}^{\text{peq}}(r_b, t) + \tilde{\epsilon}_i \tilde{n}_{i,U}^{\text{peq}}(r_b, t) \). With Equation (13), energy conservation determines \( \theta^{\text{eff}} \), which itself contains the link bounce back phonon collision scheme:

\[
\theta^{\text{eff}} = \frac{\epsilon_j n_j(r, t) - \epsilon_j w_j A_j + \tilde{\epsilon}_j \tilde{n}_j(r + c_i \Delta t, t) - \tilde{\epsilon}_i \tilde{w}_i \tilde{A}_i}{\beta_0 \left( w_j (\epsilon_j)^2 B_j + w_i (\tilde{\epsilon}_i)^2 \tilde{B}_i \right)}.
\] (14)

It is worth noting that \( \theta^{\text{eff}} \) is in general different from the average temperature of two lattice nodes linked by the boundary node, unless the same dispersion relation is shared by the two lattice nodes. If the average temperature were to be used in place of \( \theta^{\text{eff}} \), the energy conservation principle would be violated; the interface would end up pumping in or sinking out a certain amount of energy to or from the system through the collision process.

When \( \lambda_I = 2 \), i.e. \( \tau_I = 0.5 \Delta t \), in Equation (12), the post-collision energy is distributed proportionally to the heat capacity of the two phonon phases. This condition corresponds to the diffusive mismatch model of the interface thermal resistance, which reproduces the zero interface thermal resistance in the macroscopic limit. Essentially, the pseudo-equilibrium distribution is what is used to simulate the diffusive mismatch model in the LBPC equation.

3. Discussion

The phonon mean free path is an important parameter directly affecting the heat conductivity (or conductance) of the system. Therefore, it is possible to have a system composed of separate regions of different heat conductivities by assigning different relaxation times to each region [22]. Such a system has inhomogeneous heat conductivity but homogeneous heat capacity as long as the phonons of different regions share the same dispersion relation, hence thermal equilibrium indicates an equal amount of energy across the regional boundary. In many important applications of nanocomposites and multilayered devices, thermal interfaces are usually between materials of different heat conductivities and also of different heat capacities. In such cases, the interface thermal resistance needs to be included in the model. In this section, using results attained from the D3Q19 LBPC model, we discuss how the finite phonon mean free path and the interface thermal resistance are determined by \( \tau_U \) and \( \tau_I \) of Equations (4) and (11).
3.1. Phonon mean free path, $\Lambda$

The phonon mean free path may have a multitude of meanings. It may refer to the mean distance of phonon propagation between successive Umklapp collisions. A convenient definition of the phonon mean free path for the Callaway collision operator is the distance a phonon travels during the linear relaxation time, $\Lambda_U = v_g \tau_U$. It refers to the momentum screening length over which the phonon momentum correlation decays exponentially, considering that the Umklapp collision process does not conserve the phonon momentum.

In the LBPC equation, however, where the time domain is discretized by $\Delta t$, this definition is valid only when $\tau_U/\Delta t$ is large, because the linear relaxation time loses its physical basis as $\tau_U$ approaches $\Delta t$. This issue becomes easy to understand with the case when $\tau_U = \Delta t$. In the BPC formalism, any non-equilibrium phonon distribution exponentially relaxes to the local equilibrium distribution in the finite time-scale of $\tau_U$. However, in the LBPC formalism, because $\Delta t$ is the time unit of the LBPC equation, $\tau_U$ of $\Delta t$ implies an immediate relaxation and zero mean free path.

An alternative definition of the phonon mean free path, physically meaningful even at small $\tau_U/\Delta t$, can be derived from the conductivity measurement using the LBPC model. The thermal conductivity, $\kappa$, is a material property definable in the limit of small Knudson number, $Kn = \Lambda/L$, where $L$ is the characteristic size of the material sample. For a fixed $\tau_U$ and variable $L$, $\kappa$ increases with $L$, and converges to $\kappa_\infty$ asymptotically at large $L$. If the autocorrelation of the phonon momentum decays exponentially, so that the screening length can be defined, then the thermal conductivity of a sample can be approximated as

$$\kappa = \frac{\kappa_\infty L}{L + \Lambda_{\text{eff}}},$$

where the momentum screening length, $\Lambda_{\text{eff}}$, is the effective phonon mean free path. When $L \gg \Lambda_{\text{eff}}$, $\kappa$ asymptotically converges to $\kappa_\infty$, the material property of the sample. When $L \ll \Lambda_{\text{eff}}$, $\kappa$ becomes proportional to $L$, as expected in the phonon dynamics without Umklapp collision. As Equation (15), when reverted, yields

$$\frac{\kappa_\infty}{\kappa} = \frac{\Lambda_{\text{eff}} \Delta x}{\Delta x L} + 1,$$

$\Lambda_{\text{eff}}$ can be deduced from a series of $\kappa$ measurements of samples with a fixed $\tau_U$ and varying $L$. The measurement of $\kappa$ is performed in the following procedure. For a given system with a fixed $\tau_U$, a finite temperature difference, $\Delta \theta$, is applied on two opposite faces separated by $L$ using the Planck distribution. The heat flux is measured, then divided by $\Delta \theta/L$ to give $\kappa$. Figure 3(a) shows that such measurements produce a linear relation between $\kappa^{-1}$ and $L^{-1}$ as Equation (16). $\Lambda_{\text{eff}}$ is given by the slope of the linearity, while the $y$-intercept yields $\kappa_\infty$, the thermal conductivity as the material property of the sample.

As discussed above, $\Lambda_U$, in the BPC equation, is a valid and convenient definition of the phonon mean free path based on $\tau_U$. However, the discrete time domain of the LBPC formalism makes $\Lambda_U$ obsolete for small $\tau_U/\Delta t$. On the other hand, $\Lambda_{\text{eff}}$ is the physical screening length of the phonon momentum in the LBPC formalism. Those two definitions of the phonon mean free path are compared in Figure 3(b) over a broad range of $\tau_U$. At large $\tau_U/\Delta t$, $\Lambda_U$ is a valid definition of the phonon mean free path of the LBPC model, quantitatively agreeing with $\Lambda_{\text{eff}}$. However, as $\tau_U$ approaches $\Delta t$, $\Lambda_U$ overestimates the actual screening length which diminishes at $\tau_U = \Delta t$. 
3.2. Interface thermal resistance, $\rho$

The existence of an interface usually results in an increased thermal resistance at the interface. The poor heat flux across the interface, normally signified by a finite drop or jump in the temperature profile across the interface, is qualitatively ascribed to the mismatch in the vibration density of states between two neighboring materials [34]. Figure 4(a) shows an example of a simple hetero-interface between two different phonon phases A and B. When such a system is placed between thermal reservoirs at two different temperatures at $x = 0$ and $x = L$, the interface thermal resistance results in a finite temperature drop, $\Delta \theta_I$, at the interface, as shown in Figure 4(b). The ratio of $\Delta \theta_I$ to the heat flux across the interface is the interfacial thermal resistance, $\rho$, also known as the Kapitza resistance. A length-scale called the Kapitza length is conveniently associated as an indicator of the thermal resistance. In the example shown in Figure 4(b), the Kapitza length, $h_A$, is calculated based on the temperature slope in phase A. The physical interpretation of $h_A$ is that the amount of resistance to the heat flux at the interface is comparable to that coming from the bulk phase A of thickness $h_A$. 

Figure 3. (a) The thermal conductivity ($\kappa$) measured while changing the system size ($L$) with a fixed $\tau_U$. From the slope of the dotted line, $\Lambda_{\text{eff}}$ is measured to be $14.5 \Delta x$ when $\tau_U = 16 \Delta t$. (b) The effective phonon mean free paths ($\Lambda_{\text{eff}}$) are plotted against the Umklapp collision relaxation time ($\tau_U$).
Figure 4. (a) A schematic of the simulation setting. A and B denote different phonon phases. An interface exists between phase A and phase B. A constant-temperature boundary condition is applied at \(x = 0\) and \(x = L\), so that the heat flux is established along the \(x\)-direction. (b) An example of the steady state temperature profile developed from setting (a) to illustrate the interface resistance. A finite temperature drop at the interface occurs as a result of the finite resistance at the interface. \(h_A\) is the length covered by the extension of the temperature profile in phase A to cover the finite temperature drop at the interface.

The relation between \(\rho\) and \(\tau_I\) of the link bounce back phonon collision rule has been thoroughly tested for interfaces between two phonon phases when the bulk phonon dynamics are dominated by Umklapp processes in both phases [25]. Here, we test the interface collision rule when the bulk phonon collision dynamics in one of those two phases facing each other at the interface is dominantly governed by the normal process. The test is done in the setting shown in Figure 4 using the D3Q19 LB model, where the Umklapp process dominates in phase A. In this simple one-dimensional setting, where the heat flux along the \(x\)-direction is normal to the planar interfaces, \(\rho\) and \(h\) can be defined unambiguously.

The measurement of \(h_A\) follows the scheme shown in Figure 4(b). For a given boundary condition and the phonon properties of phase A and phase B, the temperature profile is measured. Then, from the slope of the temperature profile in phase A and the measured temperature drop at the interface, \(\Delta \theta_I\), \(h_A\) is calculated. Because the bulk phonon dynamics of phase A is dominated by the Umklapp process, \(\kappa_A\) is a material property independent of the thickness of phase A. \(\rho\) is linearly proportional to \(h_A\); \(\rho = h_A/\kappa_A\).
Figure 5. The Kapitza length \((h_A)\) plotted against the interface phonon collision relaxation time \((\tau_I)\). Solid squares are for the heat capacity case of phase B, while solid circles are for the mean free path case of phase B. To realize the interface of a given thermal resistance, different values of \(\tau_I\) should be used for different cases of phase B.

Figure 5 shows the relation between the calculated \(h_A\) and \(\tau_I\) used in the interface phonon collision. Two different cases of phase B in the middle are used for comparison. The heat conductivity as a material property of phase B, \(\kappa_B\), is 30 times larger than \(\kappa_A\) in both cases, but for different reasons. In the LBPC equation, \(\kappa_\infty\) can be directly manipulated in two independent ways. One way is to control the phonon mean free path \((\Lambda)\), and the other way is to change the heat capacity \((C)\) of the material. Although the phonon group velocity is another variable to control \(\kappa_\infty\), it is not explicitly included in the LBPC formalism introduced in this paper. In one case of phase B, which we name the “heat capacity case”, the heat capacity of phase B is 30 times larger than that of phase A, \(C_B = 30C_A\), while \(\Lambda_{\text{eff,A}}\) and \(\Lambda_{\text{eff,B}}\) are both zero. In the other case of phase B, which we name the “mean free path case”, the high heat conductivity of phase B is solely due to large mean free path, \(\Lambda_{\text{eff,B}} = 30\Delta x\). In Figure 5, we show that the Kapitza length, hence the Kapitza resistance, is linearly proportional to \(\tau_I\) in both cases of phase B, but with different proportionality for each case. It can be further shown that the phonon interface collision rule of Equation (11) realizes a local interface, whose \(\rho\) is independent of the location of the interface, the size of phase B, or other global variables of the system. Only the phonon dispersion relation of the two phases divided by the interface, the Callaway collision times of each phase, and \(\tau_I\) determine \(\rho\) at the interface [25]. This locality of \(\rho\) is a very important property of the phonon interface collision rule reviewed in this paper, because it allows a predetermined relationship between \(\rho\) and \(\tau_I\) using a simple setting as in Figure 4 to be applied to interfaces of complex shape with confidence.

We exclude from the discussion the case where the phonon mean free paths in both phases divided by the interface are large. Because such a system yields a finite \(\Delta \theta_I\) even when \(\tau_I = 0.5\Delta t\), therefore \(\Delta \theta_I\) and \(h\) are no longer indicators linearly proportional to \(\rho\). For such a system, the interface thermal resistance is poorly defined, and the microscopic description using the energy transmission coefficient is more suitable to characterize the thermal interface.

The LBPC equation can find applications in heat transfer problems where the phonon mean free path and the interface thermal resistance are non-negligible, which can be associated with most small-scale systems including thin films and nanocomposites where
Figure 6. (Color online) (a) An example configuration of a particulate composite material, where a well-separated random distribution of 2304 spherical fillers is immersed in the matrix. The volume fraction is 30%. Different shades (colors) are used for presentation purposes to distinguish particles. The system volume is $(128\Delta x)^3$ and the particle diameter is $8\Delta x$. Phase A is used for the matrix, while the “heat capacity case” phase B material is used as fillers. When $\tau_l = 0.5\Delta t$ is used to model the thermally conducting interface, the effective thermal conductivity is calculated to be $2.1\kappa_{\text{eff}}$, which quantitatively agrees with the analytic prediction of the equivalent inclusion method [40]. (b) Magnitude of the heat flux at steady state is shown on the $xy$ cross-section at $z = 0$. A temperature gradient is applied along the horizontal direction, $x$, by imposing the fixed temperature boundary condition at $x = 0\Delta x$ and $x = 128\Delta x$. The heat flux along the $x$-direction is shown as divided by the average heat flux.

materials with different mechanical and thermal properties are mixed for engineering purposes. Although a simple one-dimensional heat flux problem is used in this section, that is because $\Lambda_{\text{eff}}$ and $\rho$ can be defined unambiguously in such a setting. Actually, the phonon interface collision rule itself applies to an interface of arbitrary shape, because the collision rule is defined at each boundary nodal point which is the building block of the material interface. Figure 6 shows such an example of a three-dimensional particulate composite system, where highly conductive particulate fillers are embedded in a matrix of
poor conductivity. It is a large-scale simulation involving more than 2000 particles. The superb parallelizability of the LBPC equation and the link bounce back collision scheme can afford such large-scale simulations efficiently.

Considering the advanced knowledge and insights in the LB fluid dynamics literature, the LBPC equation for phonon dynamics has vast potential to further develop and grow in many applications. For example, LB boundary conditions studied for complex geometry flows such as porous and textile flow should facilitate the modeling of heat transfer in complex geometries like carbon forms and network structures [35, 36]. The kinetic boundary condition for LB microfluidics may inspire microscopic phonon interface collision rules [37–39].

4. Conclusions

In the sub-micro spatio-temporal scale of current interest to the device industry, heat transfer modeling needs to consider the effects of the finite phonon mean free path and the interface thermal resistance. Based on the linear relaxation of a non-equilibrium phonon distribution toward local equilibrium, the lattice Boltzmann Peierls–Callaway equation with its recently proposed mesoscopic phonon interface collision rule can realize a finite phonon mean free path and multiphase phonon gas with interface thermal resistance. In the Callaway collision operator, the Umklapp collision relaxation time, \( \tau_U \), determines the phonon mean free path, while the interface collision relaxation time, \( \tau_I \), determines the Kapitza length, hence the Kapitza resistance. The highly parallelizable LB numerical scheme enables the LBPC equation to model large-scale simulations efficiently. The emerging LBPC equation for phonon hydrodynamics is anticipated to benefit from the accumulated insights of the LB literature and develop applications in various heat transfer problems in the future.

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References

[1] W.P. Mason, Phonon viscosity and its effect on acoustic wave attenuation and dislocation motion, J. Acoust. Soc. Am. 32 (1960), pp. 458–472.
[2] M. Chester, Second sounds in solids, Phys. Rev. 131 (1963), p. 2013–2015.
[3] R.A. Guyer and J.A. Krunhansl, Solution of the linearized phonon Boltzmann equation, Phys. Rev. 148 (1966), p. 766–778.
[4] R.A. Guyer and J.A. Krunhansl, Thermal conductivity, second sound, and phonon hydrodynamic phenomena in nonmetallic crystals, Phys. Rev. 148 (1966), p. 778–788.
[5] H.J. Maris, Phonon viscosity, Phys. Rev. 188 (1969), pp. 1303–1307.
[6] D. Benin, Phonon viscosity and wide-angle phonon scattering in superfluid helium, Phys. Rev. B 11 (1975), pp. 145–149.
[7] A. Majumdar, Microscale heat conduction in dielectric thin films, J. Heat Transfer 115 (1993), p. 7–16.
[8] S. Mazumder and A. Majumdar, Monte Carlo study of phonon transport in solid thin films including dispersion and polarization, J. Heat Transfer 123 (2001), p. 749–759.
[9] A. Mittal and S. Mazumder, Monte Carlo study of phonon heat conduction in silicon thin films including contributions of optical phonons, J. Heat Transfer 132 (2010), 052402.
[10] G. Chen, Thermal conductivity and ballistic-phonon transport in the cross-plane direction of superlattices, Phys. Rev. B 57 (1998), p. 14958–14973.

[11] R. Prasher, Generalized equation of phonon radiative transport, Appl. Phys. Lett. 83 (2003), p. 48–50.

[12] R.G. Yang and G. Chen, Thermal conductivity modeling of periodic two dimensional nanocomposites, Phys. Rev. B 69 (2004), 195316.

[13] R. Escobar, S.S. Ghai, M.S. Jhon, and C. Amon, Multi-length and time scale thermal transport using the lattice Boltzmann method with application to electronic cooling, Int. J. Heat Mass Transfer 49 (2006), p. 97–107.

[14] M.-S. Jeng, R. Yang, D. Song, and G. Chen, Modeling the thermal conductivity and phonon transport in nanoparticle composites using Monte Carlo simulation, J. Heat Transfer 130 (2008), 042410.

[15] R. Benzi, S. Succi, and M. Vergassola, The lattice Boltzmann equation: theory and applications, Phys. Rep. 222 (1992), p. 146–197.

[16] H. Li and H. Ki, Lattice-Boltzmann simulation of laser interaction with weakly ionized helium plasmas, Phys. Rev. E 82 (2010), 016703.

[17] C.K. Aidun and J.R. Clausen, Lattice-Boltzmann method for complex flows, Ann. Rev. Fluid Mech. 42 (2010), p. 439–472.

[18] U. Frisch, B. Hasslacher, and Y. Pomeau, Lattice gas automata for the Navier–Stokes equation, Phys. Rev. Lett. 56 (1986), pp. 1505–1508.

[19] D.A. Wolf-Gladrow, Lattice-Gas Cellular Automata and Lattice Boltzmann Models, Springer-Verlag, Berlin, 2000.

[20] S. Succi, The Lattice Boltzmann Equation for Fluid Dynamics and Beyond, Clarendon Press, Oxford, 2001.

[21] R.A. Guyer, Phonon gas: A lattice Boltzmann description, Phys. Rev. E 50 (1994), p. 4596–4608.

[22] W.-S. Jiaung and J.-R. Ho, Lattice-Boltzmann modeling of phonon hydrodynamics, Phys. Rev. E 77 (2008), 066710.

[23] W.-S. Jiaung and J.-R. Ho, Lattice Boltzmann study on size effect with geometrical bending on phonon heat conduction in a nanoduct, J. Appl. Phys. 95 (2004), p. 958–966.

[24] A.J.C. Ladd, Numerical simulations of particulate suspensions via a discretized Boltzmann equation, Part I. Theoretical foundation, J. Fluid. Mech. 271 (1994), p. 285–310.

[25] J. Lee, A.K. Roy, and B.L. Farmer, Kapitza resistance in the lattice-Boltzmann–Peierls–Callaway equation for multiphase phonon gases, Phys. Rev. E 83 (2011), 056706.

[26] J.M. Ziman, Electrons and Phonons: The Theory of Transport Phenomena in Solids, Oxford University Press, London, 1960.

[27] J. Callaway, Model for lattice thermal conductivity at low temperature, Phys. Rev. 113 (1959), p. 1046–1051.

[28] G.L. Pollack, Kapitza resistance, Rev. Mod. Phys. 41 (1969), pp. 48–81.

[29] P.L. Bhatnagar, E.P. Gross, and M. Krook, A model for collision processes in gases. I. Small amplitude processes in charged and neutral one-component systems, Phys. Rev. 94 (1954), p. 511–525.

[30] A.J.C. Ladd and R. Verberg, Lattice-Boltzmann simulations of particle-fluid suspension, J. Stat. Phys. 104 (2001), p. 1191–1251.

[31] T. Yamamoto and K. Watanabe, Nonequilibrium Green’s function approach to phonon transport in defective carbon nanotubes, Phys. Rev. Lett. 96 (2006), 255503.

[32] N. Mingo, D.A. Stewart, D.A. Broido, and D. Srivastava, Phonon transmission through defects in carbon nanotubes from first principles, Phys. Rev. B 77 (2008), 033418.

[33] J. Wang and J.S. Wang, Single-mode phonon transmission in symmetry-broken carbon nanotubes: Role of phonon symmetry, J. Appl. Phys. 105 (2009), 063509.

[34] E.T. Swartz and R.O. Pohl, Thermal boundary resistance, Rev. Mod. Phys. 61 (1989), p. 605–668.

[35] C. Pan, L.-S. Luo, and C.T. Miller, An evaluation of lattice Boltzmann schemes for porous medium flow simulation, Comput. Fluids 35 (2006), p. 898–909; doi=10.1016/j.compfluid.2005.03.008.

[36] B. Ahrenholz, J. Tölke, and M. Krafczyk, Lattice-Boltzmann simulations in reconstructed parametrized porous media, Int. J. Comp. Fluid Dynam. 20 (2006), p. 369–377; doi=10.1080/10618560601024694.
[37] S. Succi, *Mesoscopic modeling of slip motion at fluid–solid interfaces with heterogeneous catalysis*, Phys. Rev. Lett. 89 (2002), 064502.

[38] S. Ansumali and I.V. Karlin, *Kinetic boundary conditions in the lattice Boltzmann method*, Phys. Rev. E 66 (2002), 026311.

[39] M. Sbragaglia and S. Succi, *Analytical calculation of slip flow in lattice Boltzmann models with kinetic boundary conditions*, Phys. Fluids 17 (2005), 093602.

[40] H. Hatta and M. Taya, *Effective thermal conductivity of a misoriented short fiber composite*, J. Appl. Phys 58 (1985), p. 2478–2486.