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Large-scale parallel computation of the phonon Boltzmann Transport Equation

Syed Ashraf Ali [a], Gautham Kollu [b], Sandip Mazumder [a, *], P. Sadayappan [b], Arpit Mittal [a]

[a] Department of Mechanical and Aerospace Engineering, The Ohio State University, Columbus, OH 43210, USA
[b] Department of Computer Science and Engineering, The Ohio State University, Columbus, OH 43210, USA

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ABSTRACT

Non-equilibrium heat conduction, as occurring in modern-day sub-micron semiconductor devices, can be predicted effectively using the Boltzmann Transport Equation (BTE) for phonons. In this article, strategies and algorithms for large-scale parallel computation of the phonon BTE are presented. An unstructured finite volume method for spatial discretization is coupled with the control angle discrete ordinates method for angular discretization. The single-time relaxation approximation is used to treat phonon–phonon scattering. Both dispersion and polarization of the phonons are accounted for. Three different parallelization strategies are explored: (a) band-based, (b) direction-based, and (c) hybrid band/cell-based. Subsequent to validation studies in which silicon thin-film thermal conductivity was successfully predicted, transient simulations of non-equilibrium thermal transport were conducted in a three-dimensional device-like silicon structure, discretized using 604,054 tetrahedral cells. The angular space was discretized using 400 angles, and the spectral space was discretized into 40 spectral intervals (bands). This resulted in ~9.7×10^9 unknowns, which are approximately 3 orders of magnitude larger than previously reported computations in this area. Studies showed that direction-based and hybrid band/cell-based parallelization strategies resulted in similar total computational time. However, the parallel efficiency of the hybrid band/cell-based strategy—about 88%—was found to be superior to that of the direction-based strategy, and is recommended as the preferred strategy for even larger scale computations.

1. Introduction

Overheating is one of the most common causes of semiconductor device failure. The POWER7, launched in early 2010, contains 1.2 billion transistors on a single processor and dissipates about 100 W/cm^2. As VLSI technology scales, thermal issues are becoming the dominant factor in determining performance, reliability, and cost of high-performance integrated circuits. According to the International Technology Roadmap for Semiconductors (I.T.R.S) published in 2012 [1], understanding of fundamental physical mechanisms underlying thermal transport at the device scale is critical to the development of heat removal strategies. Therefore, modeling of thermal transport at the device scale can be beneficial in shedding light on the physical mechanisms at play.

The mean free path of the energy-carrying acoustic wave packets (or phonons) in silicon at room temperature is approximately 300 nm [2]. On the other hand, characteristic dimensions of modern semiconductor devices range from a few tens of nanometers to a few hundreds of nanometers [1–3]. Consequently, heat conduction in such devices cannot be described adequately using continuum equations, namely the Fourier law of heat conduction. The Boltzmann Transport Equation (BTE) for phonons has been used successfully in the past for the prediction of non-equilibrium heat conduction phenomena, and continues to be popular because of its validity over a large range of length scales [3].

The BTE is a seven-dimensional nonlinear integro-differential equation: 3 spatial coordinates, 3 wavevector coordinates, and time. Even in its linearized form (*i.e.*, under the so-called single relaxation time approximation), it is a seven-dimensional partial differential equation. Thus, its solution is quite challenging. The existing literature on the solution of the BTE for phonon transport reveals that there are essentially three methods that have been employed to date to solve the BTE: (a) the Monte Carlo method, (b) the Lattice Boltzmann Method, and (c) deterministic discretization-

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

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based methods. While the Monte Carlo method is amenable for the inclusion of complex physics such as dispersion, polarization, boundary scattering *etc.*, as originally demonstrated by Mazumder and Majumdar [4] and subsequently used by several researchers [5,6], it is prohibitively expensive for practical engineering applications. In recent years, variance reduction techniques have enabled use of the Monte Carlo method for solution of the BTE in somewhat realistic three-dimensional structures [7]. The lattice Boltzmann method has only been used for the solution of the phonon BTE in simple two-dimensional structures [8,9]. Deterministic solution of the BTE has its early roots in neutron and radiation (photon) transport, and has been brought to the limelight for phonon transport primarily by Murthy and co-workers [10–13]. Some research has also been conducted by the same researchers on hybridizing BTE-based models with continuum (Fourier-based) models [14]. Much of the work on deterministic solution of the BTE, however, has only been demonstrated for relatively simple two-dimensional structures and/or steady state. Recently, Mittal and Mazumder [15–17] have demonstrated solution of the unsteady gray BTE in large-scale three-dimensional structures with about 400,000 grid points and 400 directions. To the best of the authors' knowledge, to date, the unsteady solution of the phonon BTE with the inclusion of dispersion and polarization using deterministic methods has only been demonstrated in regular Cartesian one- and two-dimensional structures [10–14,18–20]. This is because such computations are challenging both from a memory as well as computational time standpoint.

To bring to light the magnitude of the computational challenge that has to be overcome to solve the unsteady phonon BTE with the inclusion of dispersion and polarization effects, it is instructive to conduct a back-of-the-envelope estimate. It is estimated that the solution of the BTE in a practical device, such as a transistor, will arguably require ~5 M nodes or cells to adequately resolve all the relevant length scales and obtain grid-independent solutions. To date, deterministic solution of the BTE with the inclusion of dispersion and polarization has only been conducted in simplified two-dimensional geometries with only ~10^4 nodes or cells [19]. Since the BTE is a directional equation, discretization in two additional independent angular spaces (polar and azimuthal angles) is necessary. Typically, for 3D calculations, about 20 × 20 ($\theta \times \psi$) angular resolution is necessary to obtain angular grid independence [15,16]. Finally, when dispersion and polarization are considered, the phonon frequency (or wavevector) space must be discretized into ~100 spectral intervals or bands [17,20]. This results in ~2×10^{11} unknowns, which requires approximately 1600 GB of runtime memory just to store the unknowns in double precision. Thus, from a memory perspective alone, solution of the non-gray BTE for practical semiconductor devices will require massive parallelization.

The afore-mentioned challenge in solution of the phonon BTE has not been previously encountered in the solution of the radiative transfer equation (RTE), although it is almost identical in form to the phonon BTE. This is because of one fundamental difference. For most terrestrial applications, the RTE is solved in its steady-state form. The time-scales for light transport are so fast compared to other processes (such as fluid flow or chemical reactions), that for all practical purposes, the radiation field may be assumed to attain steady state almost instantaneously. In this scenario, the entire intensity array does not have to be stored. The contributions of the various bands and directions (at least in the case when in-scattering is neglected) can be cumulatively added to obtain the net heat flux or its divergence. In the case of the phonon BTE, the unsteady equation must be solved, because for most applications, the temporal evolution of the temperature field is of interest. Since initial conditions for each directional and spectral intensity must be provided, there is no alternative to storing the entire intensity array, making phonon BTE computations orders of magnitude more memory intensive than RTE computations.

Another challenge is the computational time required to perform such calculations. Depending on the time-step size, and the solvers used, it may take between 10 and 20 iterations to attain 3–4 orders of magnitude convergence within each time step. The iterations are necessary to couple the BTE with the overall energy equation, and to couple the directional BTEs. Thus, for a single time step, assuming that matrix-vector multiplication is the dominant process (such as in the case of Krylov sub-space solvers) for determining floating point operations (flops), the number of flops needed per time step is $5 \times 106 \times 20 \times 20 \times 100 \times 10 \times 6 = 1.2 \times 10^{13}$, where the number 6, for example, denotes the number of neighbors of each cell (*e.g.*, in a hexahedral 3D mesh). Typically, most engineering calculations of this nature require execution of between 10^3–10^4 time steps to reach steady state or to extract meaningful time-dependent physical quantities. Therefore, a computation of this type will require ~10^{17} floating point operations. To bring these numbers into perspective, to the best of the authors' knowledge, the largest reported parallel computation in this area is the one by Ni and Murthy [20] who performed calculations on a 2D rectangular domain with 80 × 80 cells, 64 angles, and 80 spectral bands, resulting in ~3×10^7 unknowns (compared to the estimated ~2×10^{11} unknowns for practical semiconductor device computations). The present work attempts to close the gap between the state-of-the-art and the ultimate goal. Its contribution lies in presenting and demonstrating a scalable algorithm for parallel computation of the phonon BTE for test problems that are several orders of magnitude larger than previously reported studies in this area.

2. Theory and mathematical formulation

Quantized lattice vibrations or phonons are the predominant carriers of thermal energy in semiconductor materials [21]. 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. Heat conduction, in such a scenario, is referred to as non-equilibrium heat conduction. The Boltzmann Transport Equation for phonons has found prolific usage in the prediction of non-equilibrium heat conduction in semiconductor materials.

2.1. Boltzmann Transport Equation

The Boltzmann Transport Equation (BTE) has been successfully used to model phonon transport. Under the single-time relaxation approximation, the BTE for phonons becomes a linear partial differential equation, and may be written as [3]

$$\frac{\partial f}{\partial t} + \upsilon_g \cdot \nabla f = \frac{f_0 - f}{\tau} \tag{1}$$

where f is the distribution function of an ensemble of phonons, f_0 is the equilibrium number density function (*i.e.*, the Bose–Einstein distribution function), τ is the overall scattering time-scale of the phonon due to all scattering processes in combination, and υ_g is the group velocity. The left side of Eq. (1) represents change in 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.

For an isotropic wavevector space, the distribution function, f, is a function of seven independent variables, *i.e.*, $f = f(t, \mathbf{r}, \hat{\mathbf{s}}, \omega)$, where t is time, and ω is the angular frequency. The space vector $\mathbf{r}$