Finite Element Analysis of Transient Ballistic-Diffusive Heat Transfer in Two-Dimensional Structures

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Abstract

For the last two centuries, the conventional Fourier heat conduction equation has been used for modeling a diffusive nature of macroscale heat conduction by considering the energy conservation and Fourier's linear approximation of heat flux. However, it cannot accurately predict heat transport when the length scale is comparable to or smaller than the mean free path of thermal energy carriers or when the time scale is shorter than the carrier relaxation time [1-5]. As microelectronic devices keep shrinking below the mean free path of thermal energy carriers, fundamental understanding of sub-continuum heat conduction becomes critically important for the effective power management and reliable operations.

For the phonon-dominant thermal energy transport, the Boltzmann transport equation (BTE) has shown promising results in predicting the ballistic-diffusive nature of heat transfer and temperature distribution [5-10]. Many numerical models have been developed to accurately compute the BTE in various multi-dimensional geometries. Such methods include the finite volume method (FVM) [11-13,15-17], the finite element analysis (FEA) [18-20], and the finite difference method (FDM) [7,8,14,21], combined with the discrete ordinate method (DOM) for angular discretization. In addition, the ballistic-diffusive approximation of the BTE has been introduced to alleviate computational complexities in directly solving the BTE while conveying the ballistic-diffusive features of phonon heat transport [21-24]. However, these methods are not widely available to general public, including undergraduate and graduate students who are not familiar with sub-continuum heat transfer, mainly due to the complexities in numerical modeling of the BTE. In order to address this challenge, we make use of a commercially available finite element method (FEM) package to compute the BTE based on the gray relaxation-time approximation.

Using COMSOL Multiphysics® software, PDE (partial differential equation) interfaces are used to define the BTE governing equation. In this study, the discrete ordinate method (DOM) is implemented to discretize the BTE in angular directions using multiple PDE modules while it is spatially discretized by the FEM. This method is validated by comparing the FEM results for a long rectangular geometry with the 1D analytic solution of phonon radiative transfer (EPRT) (fig. 1) as well as 2D ballistic-diffusive equation and finite difference solution for BTE (fig. 2).

Various multi-dimensional geometries will be considered to investigate the ballistic behavior of heat conduction and the boundary scattering effect (fig. 3). The ray effect will also be discussed as the biggest error source in obtaining accurate solution. This is done by using different numbers of PDE equations, i.e. 4 equations up to 256 equations (fig. 4). By defining appropriate terms for Dirichlet boundary conditions, we were able to solve the problem for both heating boundaries and boundaries with constant temperature. The success of this study will provide a reliable engineering tool in computing ballistic-diffusive heat conduction in micro/nanostructures.

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Figures used in the abstract

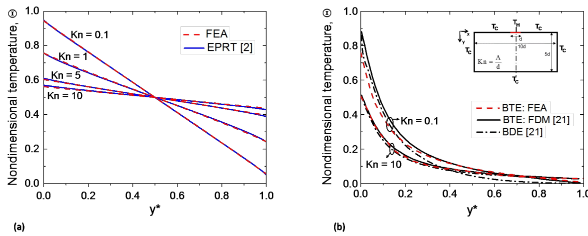

Figure 1: (a) Nondimensional temperature distribution along its center line of the rectangular domain with a high aspect ratio. Temperature distribution is normalized using the hot and cold boundaries, i.e., . To validate the model, the computation results are compared with the semi-analytical solution of the 1-D equation of phonon radiative transfer (EPRT) [2]. (b) Temperature distribution along the centerline of the rectangular domain illustrated in the inset. Results are compared with BTE-FDM and BDE from ref. [21] for further validation.

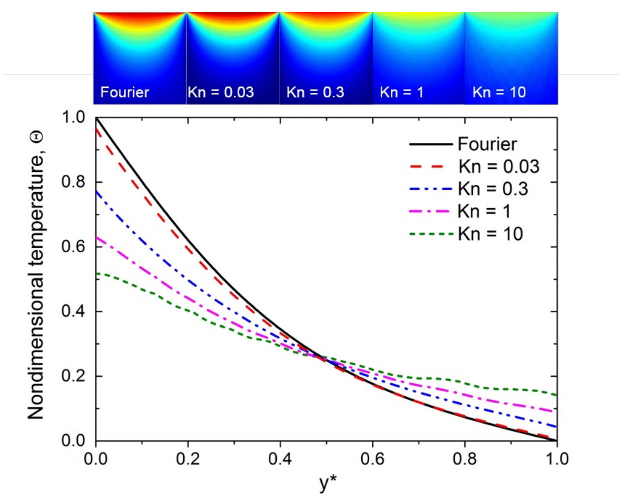

Figure 2: Nondimensional temperature distribution predicted with the BTE for different Kn numbers. For comparison, nondimensional temperature distribution predicted with the Fourier heat conduction equation is also plotted.

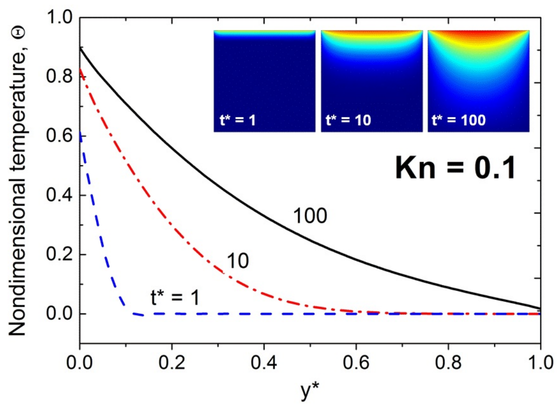

Figure 3: Transient nondimensional temperature changes along the centerline of the square domain computed by the BTE simulation for Kn = 0.1.

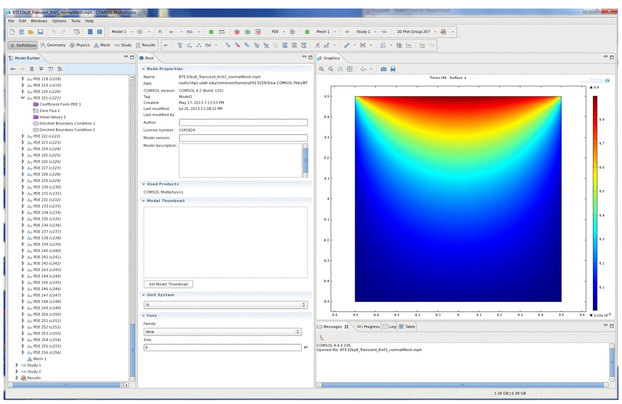

Figure 4: COMSOL snapshot for Kn = 0.1.