Nanoscale Heat Transfer using Phonon Boltzmann Transport Equation

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Outline

• Background information.

• Description of phonon Boltzmann transport equation (BTE).

• Modeling and solution procedure of BTE using COMSOL.

• Results
  – Steady-state and transient problems.
  – Issues of refinement in spatial and angular domains.

• Summary and conclusions.
For last two centuries, heat conduction has been modeled by Fourier Eq (FE).

- Conservation of energy:
  \[ \rho c \frac{\partial T}{\partial t} = -\nabla \cdot q \]

- Fourier’s linear approximation of heat flux:
  \[ q = -k\nabla T \]

\[ \frac{1}{\alpha} \frac{\partial T}{\partial t} = \nabla^2 T \]

- Parabolic equation —> Diffusive nature of heat transport.
- Heat is effectively transferred between localized regions through sufficient scattering events of phonons within medium.
- Does not hold when number of scattering is negligible.
  - e.g., mean free path \( \sim \) device size (chip-package level).
  - Boundary scattering at interfaces causing thermal resistance.
- Admits infinite speed of heat transport —> Contradict with theory of relativity.

\[ \text{Fourier Equation cannot be used for small time and spatial scales.} \]
Hyperbolic Heat Conduction Equation (HHCE)

- Resolve the issue of the Fourier equation with the infinite speed of heat carrier.
  \[ \frac{1}{C^2} \frac{\partial^2 T}{\partial t^2} + \frac{1}{\alpha} \frac{\partial T}{\partial t} = \nabla^2 T \quad (C^2 = \alpha/\tau_o) \]
  - Definition of heat flux: \[ \tau_o \frac{\partial q}{\partial t} + q = -k \nabla T \], \((\tau_o : \text{relaxation time})\)

- Hyperbolic equation —> Wave nature of heat transport.
- Called as Cattaneo equation or Telegraph equation.
- Finite speed of heat carriers.
- Ad hoc approximation of heat flux definition.
- Violates 2\textsuperscript{nd} law of thermodynamics.
  - If heat source varies faster than speed of sound, heat would appear to be moving from cold to hot.

\(\text{HHCE: could be used for short time scale, but not for short spatial scale.}\)
Small Scale Heat Transport (Time & Space)

- Fourier Equation cannot be used for small time and spatial scales.
- HHCE: could be used for short time scale, but not for short spatial scale.
- Needs equations and methods for small scale simulation in terms of both time and space.
  - Molecular dynamics simulation.
    - Accurate method.
    - Computationally expensive.
    - Suitable for systems having a few atomic layers or several thousands of atoms.
    - Not suitable for device-level thermal analysis.
  - Boltzmann Transport Equation (BTE).
  - Ballistic-Diffusive Equation (BDE).
    - Similar to Cattaneo Eq. (HHCE) with a source term.
    - Derived from BTE.
    - Good approximation of BTE without internal heat source, disturbance, etc.
BTE: also called as equation of phonon radiative transfer (EPRT).

Equation for phonon distribution function:
\[
\frac{\partial f}{\partial t} + v \cdot \nabla f = \left( \frac{\partial f}{\partial t} \right)_{\text{scat}} \approx \frac{f_o - f}{\tau_o}
\]

- Can predict ballistic nature of heat transfer.
- Neglects wave-like behaviors of phonon.
  - Valid for structures larger than wavelength of phonons (~ 1 nm @ RT).

Solution methods:
- Deterministic: discrete ordinates method, spherical harmonics method.
- Statistical: Monte Carlo.

Much more efficient than MD.

Agrees well with experimental data.
Details of Boltzmann Transport Equation (BTE)

- **Phonon intensity:**
  \[ I_\omega(t, v, r) = |v| \hbar \omega f(t, v, r) D(\omega) / 4\pi \]

- **BTE becomes EPRT:**
  \[ \frac{\partial I_\omega}{\partial t} + \mathbf{v} \cdot \nabla I_\omega = \frac{I_{\omega o} - I_\omega}{\tau_\omega}, \quad I_{\omega o} = \frac{1}{4\pi} \int I_\omega d\Omega \]
  *Equilibrium phonon intensity determined by Bose-Einstein statistics*

- **For 1-D,**
  \[ \frac{\partial I_\omega}{\partial t} + v \cos \theta \frac{\partial I_\omega}{\partial x} = \frac{I_{\omega o} - I_\omega}{\tau_\omega} \]

- **For each angle (\(\theta\)), solve non-linear equation with iterations for**
  - Solving for \(I_\omega\).
  - Updating \(I_{\omega o}\).

- **Heat flux:**
  \[ q = \int_0^{\omega_D} \int_{4\pi} \Omega I_\omega \cos \theta \, d\omega \, d\Omega \]

- **Internal energy:**
  \[ u(\approx cT) = \frac{1}{4\pi} \int \hbar \omega f D(\omega) \, d\omega \, d\Omega = \int_0^{\omega_D} \int_{4\pi} \Omega I_\omega \, d\omega \, d\Omega \]
Modeling & Solution Procedure using COMSOL

\[
\frac{\partial I}{\partial t} + v \cos \theta \frac{\partial I}{\partial x} = \frac{I_o - I}{\tau_o}
\]

- Use a built-in feature of COMSOL, “Coefficient Form PDEs”.
- The spatial domain is discretized using FE mesh.
- The angular (momentum) domain is discretized using Gaussian quadrature points.
- For each angle (\(\theta\)), set up the BTE with corresponding coefficients \(\mu_i=\cos \theta_i\) and BCs (Neumann vs. Dirichlet).
- Calculate equilibrium phonon intensity \((I_o)\) by numerical integration of \((I_i)\) using Gaussian quadratures.
- Solve.
  - Direct solver (UMFPACK).
  - Max. BDF order = 1.
- Postprocess and visualize the results.
Details of Solution Procedure

- Original 1-D BTE: \[
\frac{\partial I}{\partial t} + v\mu \frac{\partial I}{\partial x} = \frac{I_o - I}{\tau_o}, \quad (\mu = \cos \theta)
\]

- Nondimensionalize with \[
t^* = \frac{t}{\tau_o}, \quad \eta = \frac{x}{L}, \quad Kn = \frac{\Lambda}{L} \quad \rightarrow \quad \frac{\partial I}{\partial t^*} + Kn \mu \frac{\partial I}{\partial \eta} + I = I_o
\]

- Split into (+) and (-) directions:
  \[
  \begin{cases}
  \frac{\partial I^+_i}{\partial t^*} + Kn \mu_i \frac{\partial I^+_i}{\partial \eta} + I^+_i = I_o, \quad (\mu_i > 0) \\
  \frac{\partial I^-_i}{\partial t^*} + Kn \mu_i \frac{\partial I^-_i}{\partial \eta} + I^-_i = I_o, \quad (\mu_i < 0)
  \end{cases}
  \]

- Discretize angular space at Gaussian quadrature points:
  \[
  \text{Dirichlet BCs: } I^+_i \bigg|_{\eta=0} = \frac{\sigma}{\pi} T^4 \bigg|_{\eta=0}, \quad I^-_i \bigg|_{\eta=1} = \frac{\sigma}{\pi} T^4 \bigg|_{\eta=1}
  \]

- After FE run, postprocess:
  \[
  I_o(t,\eta) = \frac{1}{2} \left[ \sum_{i=1}^{n_{gp}/2} w_i I^+_i + \sum_{i=1}^{n_{gp}/2} w_i I^-_i \right]
  \]
  \[
  q(t,\eta) = 2\pi \left[ \sum_{i=1}^{n_{gp}/2} w_i \mu_i I^+_i + \sum_{i=1}^{n_{gp}/2} w_i \mu_i I^-_i \right]
  \]
Coefficient Form for BTE
(60 Finite elements, 16 Gaussian Points)
Steady-State Problem: Analytic vs. Numerical Solutions

Emissive power ~ Temperature

\[ e_0^*(\eta) = \frac{e_o(\eta) - J_{q2}^-}{J_{q1}^+ - J_{q2}^-} \]

Gradient

\[ \Delta e_0^* = e_0^*(\eta = 0) - e_0^*(\eta = 1) \]
Steady-State Problem: Analytic vs. Numerical Solutions

Heat flux

\[ q^* = \frac{q}{J_{q1}^+ - J_{q2}^-} \]

Thermal conductivity

\[ k^* = \frac{q^* L}{\Delta e_o^*} \]
Transient Problem: Effect of Spatial Refinement
(More Finite Elements)

- Refine spatial (x-) direction with \( n \) finite elements (\( n=15, 60, 120 \)).
- Divide angular direction with 16 Gaussian points (\( \text{ngp}=16 \)).

![Temperature @ \( t^*=0.1 \)]

- Spatial refinement leads to a smoother solution.
- However, it does not solve ray effect.
Transient Problem: Effect of Angular Refinement
(More Gaussian Points)

- Refine spatial (x-) direction with 240 FE elements.
- Divide angular direction with \( ngp \) Gaussian points (\( ngp=4,8,16,32,64,128 \)).

Temperature @ \( t^*=0.1 \)

- Angular refinement resolve ray effect.
- Spatial and angular refinements are independent.
- Highly refined spatial mesh with coarse angular mesh alleviates solution.
Results of BTE
(Temperature & Heat Flux Distributions with Time Increase)
Comparisons of FE, HHTC, BDE vs. BTE (Temperature & Heat Flux Distributions for 3 Kn)
Summary and Conclusions

• Nanoscale simulation is conducted for phonon heat transfer using Boltzmann transport equation.
  – Phonons for dielectric, thermoelectric, semiconductor materials.
  – Electrons for metals.
  – Gas molecules for rarefied gas states.

• Numerical solution of BTE has been obtained for 1-D problem (both steady-state and transient problems).

• Temperature and heat flux distributions from the nanoscale simulation yield completely different results from the solutions from Fourier and Cattaneo equations.
  – Thermal conductivity will be different, too.