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Nanoscale Heat Transfer using Phonon Boltzmann Transport Equation

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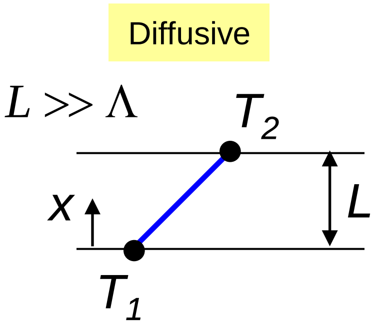
Outline

- 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.

Fourier Equation (FE)

- For last two centuries, heat conduction has been modeled by Fourier Eq (FE).
  - Conservation of energy: $\rho c \frac{\partial T}{\partial t} = -\nabla \cdot \boldsymbol{q}$
  - Fourier's linear approximation of heat flux: $\boldsymbol{q} = -k\nabla T$
  - ➢ $\frac{1}{\alpha}\frac{\partial T}{\partial t} = \nabla^2 T$



- 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 ~ device size (chip-package level).
  - Boundary scattering at interfaces causing thermal resistance.
- Admits infinite speed of heat transport —> Contradict with theory of relativity.

➢ 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.
  - ➢ $\boxed{\frac{1}{C^2}\frac{\partial^2 T}{\partial t^2}} + \frac{1}{\alpha}\frac{\partial T}{\partial t} = \nabla^2 T$ $\quad (C^2 = \alpha/\tau_o)$
  - – Definition of heat flux: $\boxed{\tau_o \frac{\partial \boldsymbol{q}}{\partial t}} + \boldsymbol{q} = -k\nabla T\ ,\quad (\tau_o : \text{relaxation time})$
- 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 2nd law of thermodynamics.
  - – If heat source varies faster than speed of sound, heat would appear to be moving from cold to hot.

➢ HHCE: could be used for short time scale, but not for short spatial scale.

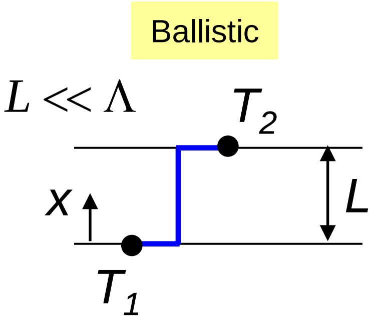
Small Scale Heat Transport (Time & Space)

- 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.

Boltzmann Transport Equation (BTE)

- BTE: also called as equation of phonon radiative transfer (EPRT).
- Equation for phonon distribution function:

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla f = \left(\frac{\partial f}{\partial t} \right)_{\mathrm{scat}} \approx \frac{f_o - f}{\tau_o}$$



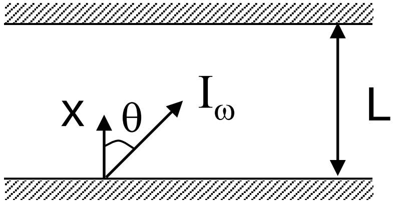
- Can predict ballistic nature of heat transfer.
- Neglects wave-like behaviors of phonon.
  - Valid for structures larger than wavelength of phonons (~ 1 nm @ RT).
- Solution methods:
  - Deterministic: discrete ordinates method, spherical harmonics method.
  - Statistical: Monte Carlo.
- Much more efficient than MD.
- Agrees well with experimental data.

Details of Boltzmann Transport Equation (BTE)

- Phonon intensity: $I_\omega(t,\boldsymbol{v},\boldsymbol{r}) = |\boldsymbol{v}|\hbar\omega f(t,\boldsymbol{v},\boldsymbol{r})D(\omega)/4\pi$

- BTE becomes EPRT: $\dfrac{\partial I_\omega}{\partial t} + \boldsymbol{v}\cdot\nabla I_\omega = \dfrac{I_{\omega o} - I_\omega}{\tau_o}$, $I_{\omega o} = \dfrac{1}{4\pi}\displaystyle\int_{\Omega=4\pi} I_\omega \, d\Omega$ *Equilibrium phonon intensity determined by Bose-Einstein statistics

- For 1-D, $\dfrac{\partial I_\omega}{\partial t} + v\cos\theta \dfrac{\partial I_\omega}{\partial x} = \dfrac{I_{\omega o} - I_\omega}{\tau_o}$



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

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

- Internal energy: $u(\approx cT) = \dfrac{1}{4\pi}\displaystyle\int \hbar\omega \, f \, D(\omega)\, d\omega \, d\Omega = \int_{\Omega=4\pi}\int_0^{\omega_D} \frac{I_\omega}{|\boldsymbol{v}|} d\omega \, d\Omega$

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 (θ), 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 $t^* = \frac{t}{\tau_o}, \quad \eta = \frac{x}{L}, \quad Kn = \frac{\Lambda}{L}$ ⇨ $$\frac{\partial I}{\partial t^*} + Kn\,\mu \frac{\partial I}{\partial \eta} + I = I_o$$

- Split into (+) and (-) directions:
- Discretize angular space at Gaussian quadrature points:

$$\begin{cases} \dfrac{\partial I_i^+}{\partial t^*} + Kn\,\mu_i \dfrac{\partial I_i^+}{\partial \eta} + I_i^+ = I_o \ , \quad (\mu_i > 0) \\ \dfrac{\partial I_i^-}{\partial t^*} + Kn\,\mu_i \dfrac{\partial I_i^-}{\partial \eta} + I_i^- = I_o \ , \quad (\mu_i < 0) \\ \text{Dirichlet BCs:}\ I_i^+\Big|_{\eta=0} = \dfrac{\sigma}{\pi} T^4\Big|_{\eta=0}, \quad I_i^-\Big|_{\eta=1} = \dfrac{\sigma}{\pi} T^4\Big|_{\eta=1} \end{cases}$$

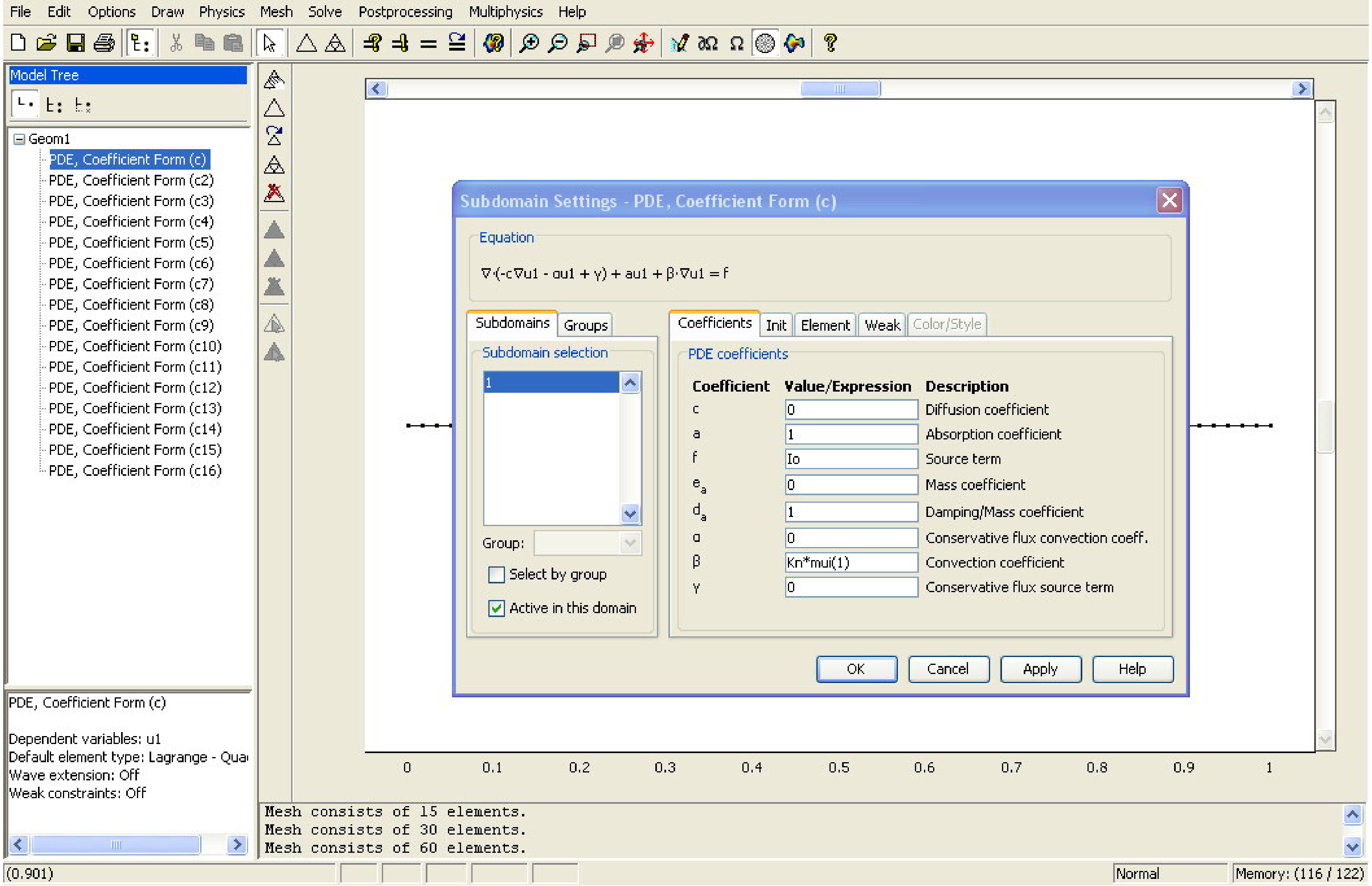
- After FE run, postprocess:

$$I_o(t,\eta) = \frac{1}{2}\left[\sum_{i=1}^{n_{gp}/2} w_i I_i^+ + \sum_{i=1}^{n_{gp}/2} w_i I_i^-\right]$$

$$q(t,\eta) = 2\pi\left[\sum_{i=1}^{n_{gp}/2} w_i \mu_i^+ I_i^+ + \sum_{i=1}^{n_{gp}/2} w_i \mu_i^- I_i^-\right]$$

Coefficient Form for BTE

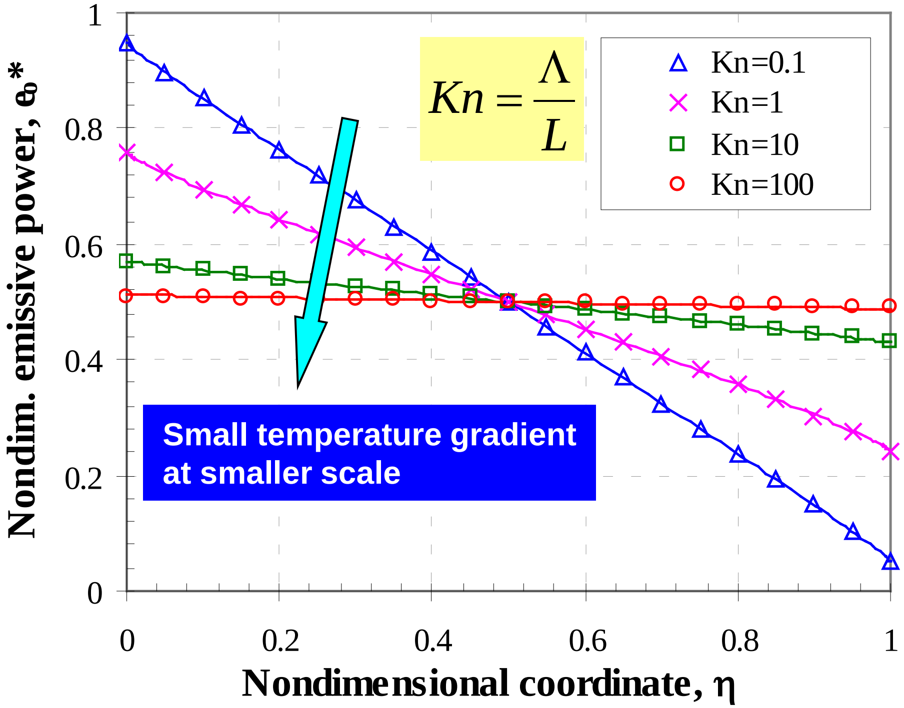
(60 Finite elements, 16 Gaussian Points)



Steady-State Problem: Analytic vs. Numerical Solutions

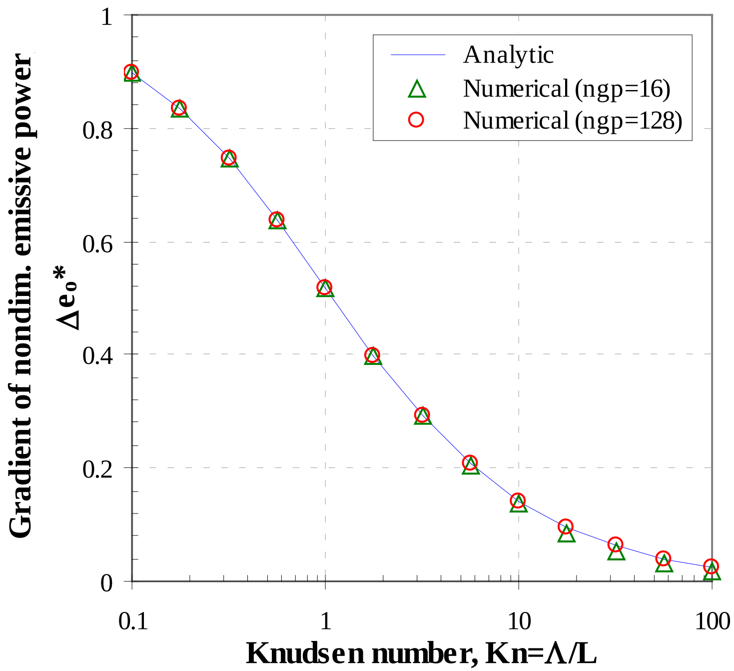
Emissive power ~ Temperature

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



Gradient

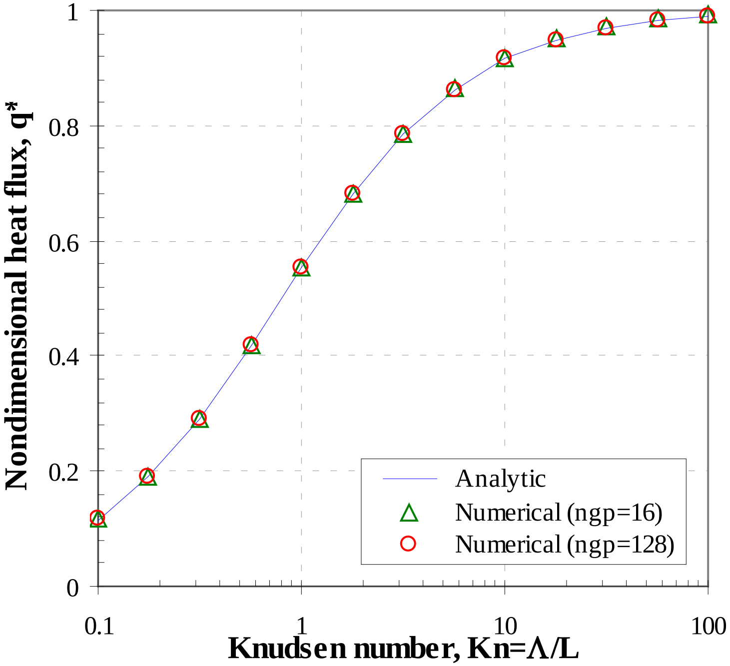
$$\Delta e_0^* = e_0^*(\eta = 0) - e_0^*(\eta = 1)$$



Steady-State Problem: Analytic vs. Numerical Solutions

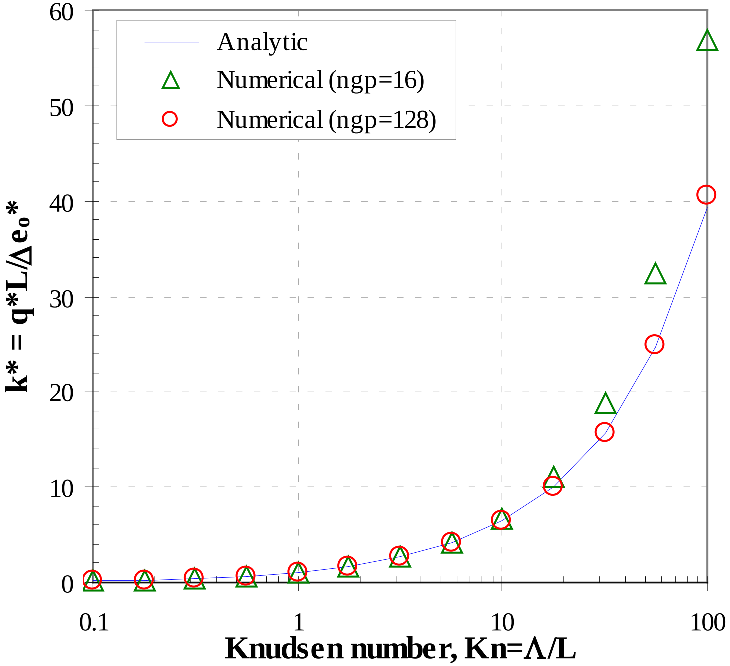
Heat flux

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



Thermal conductivity

$$k^* = \frac{q^* L}{\Delta e_o^*}$$

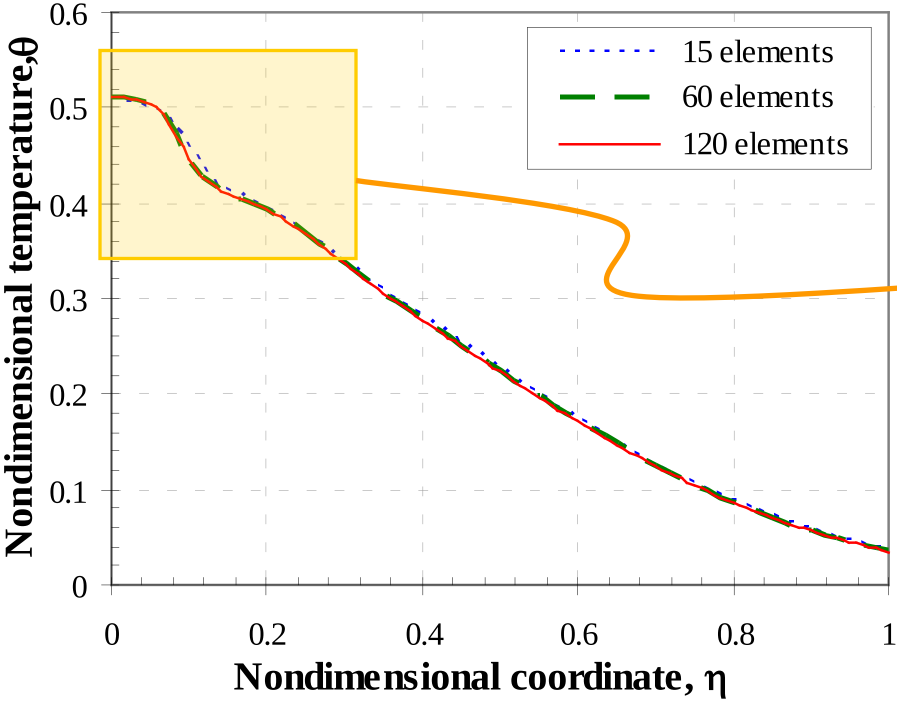


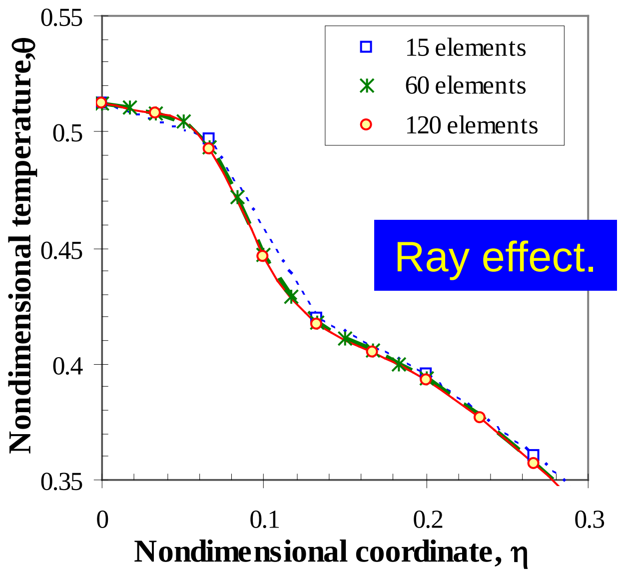
Transient Problem: Effect of Spatial Refinement

(More Finite Elements)

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

Temperature @ t*=0.1



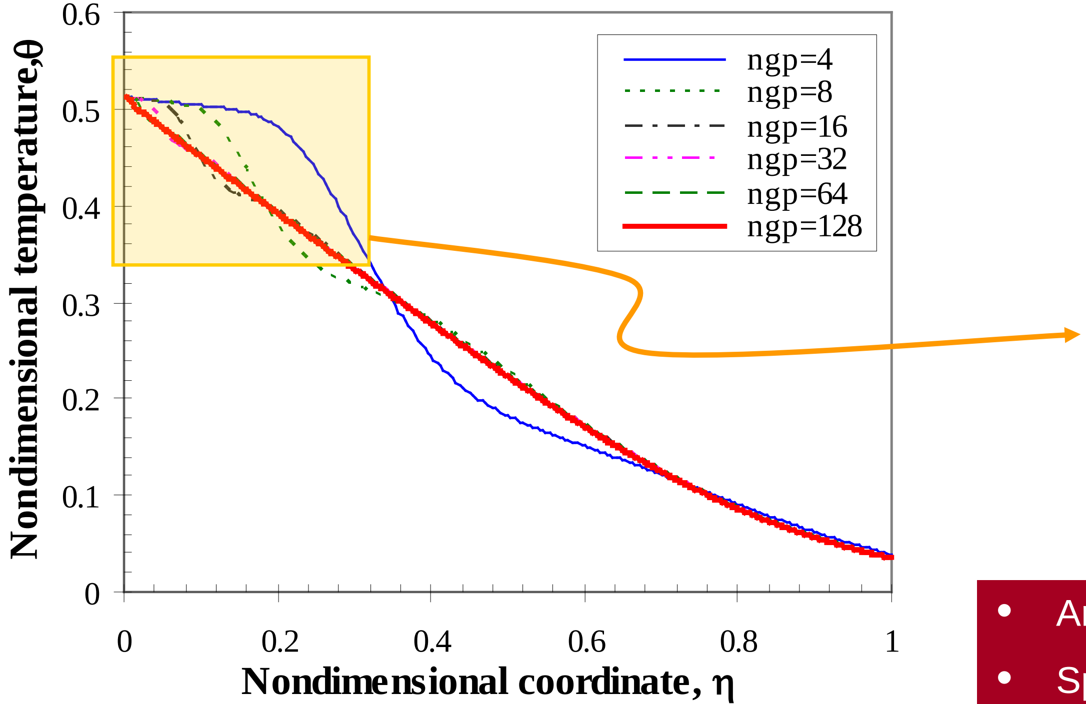


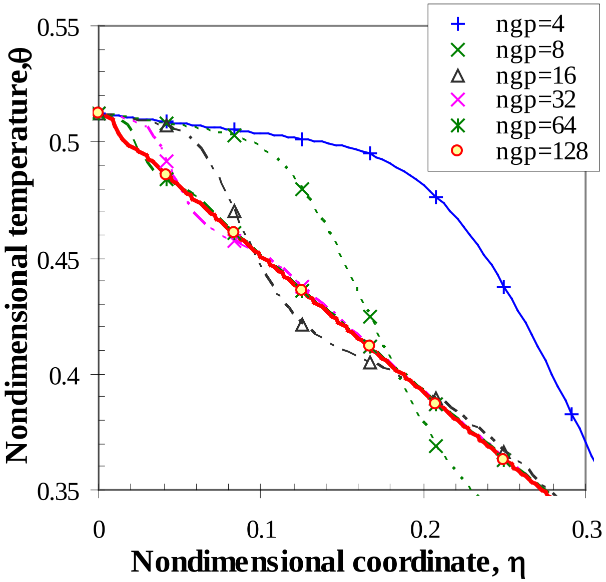
- Spatial refinement leads to a smoother solution.
- However, it does not solve ray effect.

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

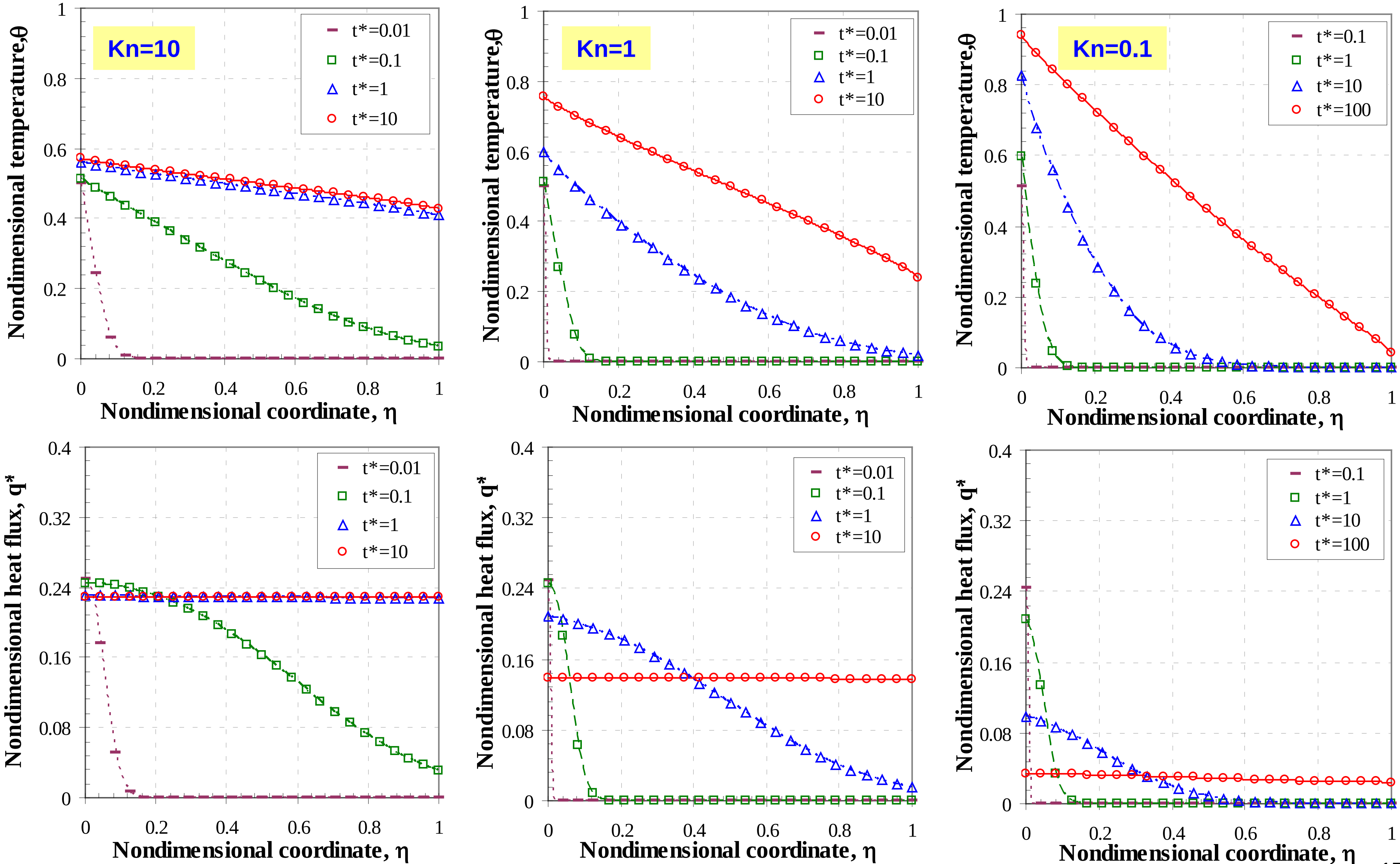




- Angular refinement resolve ray effect.
- Spatial and angular refinements are independent.
- Highly refined spatial mesh with coarse angular mesh alleviates solution.

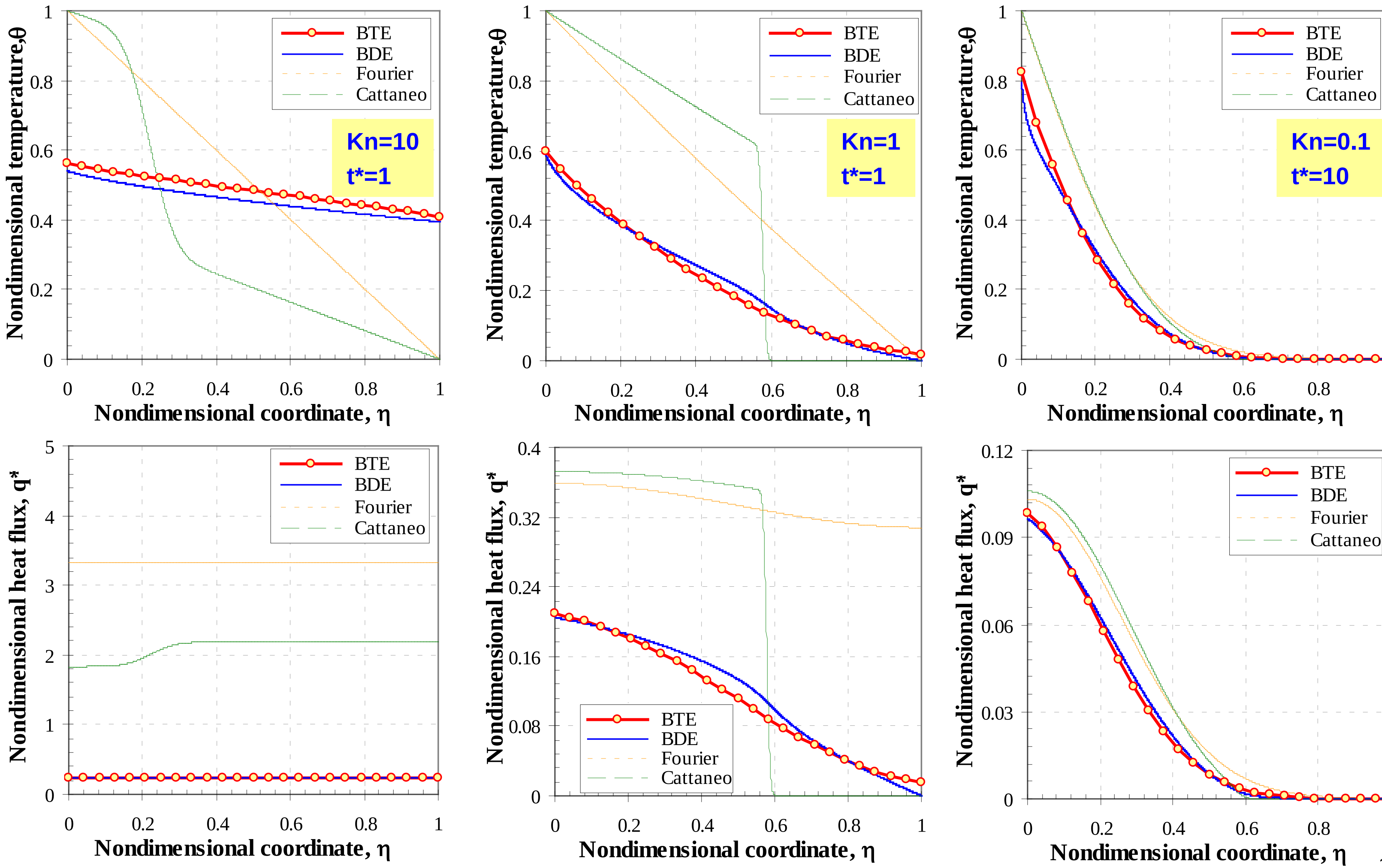
Results of BTE

(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.