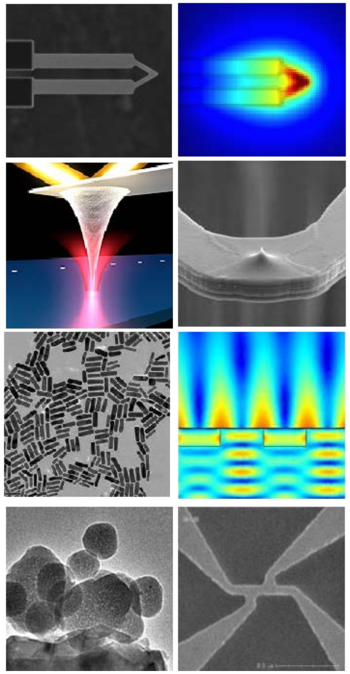
2014 COMSOL Conference, Boston, MA
October 7-9, 2014

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



Sina Hamian[1], Toru Yamada[2], Mohammad Faghri[3], and Keunhan Park[1]

1 University of Utah, Salt Lake City, UT, USA
2 Lund University, Lund, Sweden
3 University of Rhode Island, Kingston, RI, USA

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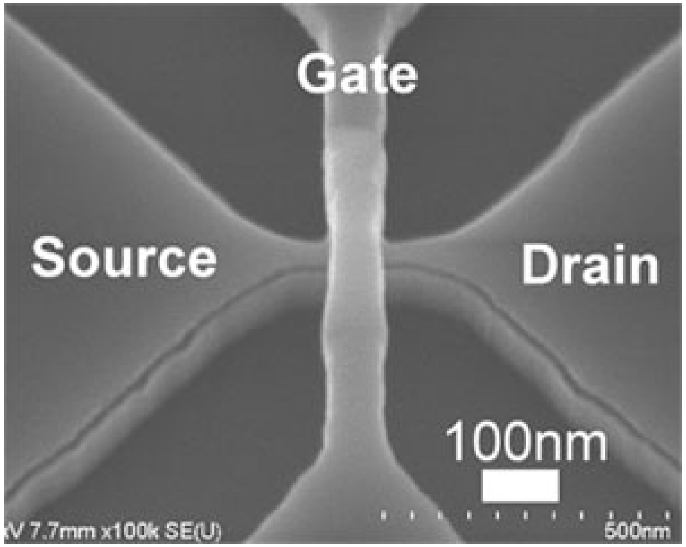
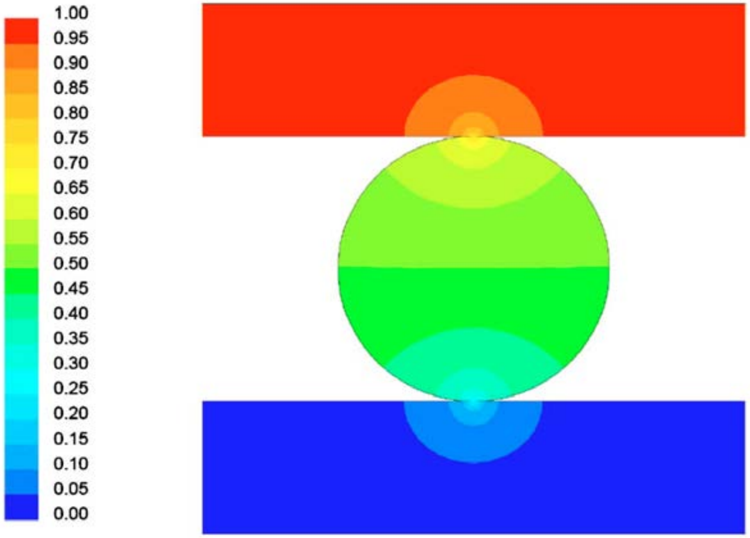
Motivation

- Size of electronic devices gets smaller and smaller such as in CPUs and transistors
- Sub-continuum heat conduction is important
- Different numerical works have been done in modeling ballistic-diffusive heat transfer
- **Not available for public in any commercial package**



An SEM image of an upright-type double-gate MOS transistor (Source: AIST)



Singh *et al.* J. of Heat Transfer, 2011

Heat transfer equations

- Fourier equation

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$$

  - Continuum medium
  - Diffusive thermal transport (Parabolic equation)
  - Cannot accurately predict sub-continuum heat transfer

- Boltzmann transport equation (BTE)
  - Based on energy carriers distribution (statistical base)
  - Complicated scattering term
  - Relaxation time approximation

$$\frac{\partial f}{\partial t} + \mathbf{v}_g \cdot \nabla f = \frac{f_0 - f}{\tau}$$

f frequency dependent distribution function

$\mathbf{v}_g$ group velocity of energy carriers

f_0 equilibrium distribution function

τ effective relaxation time

Ref: Joshi *et al.,* J. of Applied Physics, 1993

Governing equation

BTE for phonon energy density $$\frac{\partial e''}{\partial t} + \nabla \cdot (v_g \hat{\mathbf{s}} e'') = \frac{e_0'' - e''}{\tau}$$

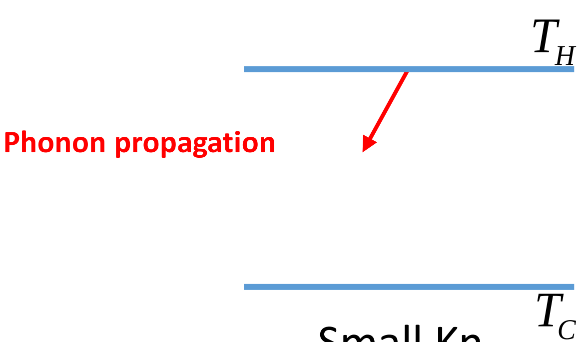
$$e''(\mathbf{r}, \hat{\mathbf{s}}, t) = \sum_p \left(\int_0^{\omega_D} D_p(\omega) f \hbar \omega d\omega \right)$$ Directional phonon energy density

$$e_0''(\mathbf{r}, t) = \frac{1}{4\pi} \int_{4\pi} e''(\mathbf{r}, \hat{\mathbf{s}}, t) d\Omega$$ Equilibrium phonon energy density

v_g Phonon group velocity

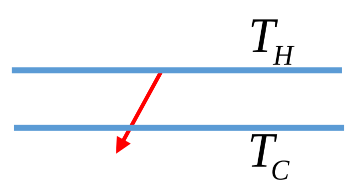
Knudsen number $$\text{Kn} = \Lambda / L$$

For a constant phonon mean free path: Smaller domain length → Larger Kn



Small Kn

$L > \Lambda$



Large Kn

$L < \Lambda$

Ref: Singh *et al.*, J. of Heat Transfer, 2011

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Nondimensional 2-D BTE + DOM

$$\frac{1}{\mathrm{Kn}}\frac{\partial e''_{n,m}}{\partial t^*}+\mu_n\frac{\partial e''_{n,m}}{\partial x^*}+\eta_{n,m}\frac{\partial e''_{n,m}}{\partial y^*}=\frac{e''_0-e''_{n,m}}{\mathrm{Kn}}$$

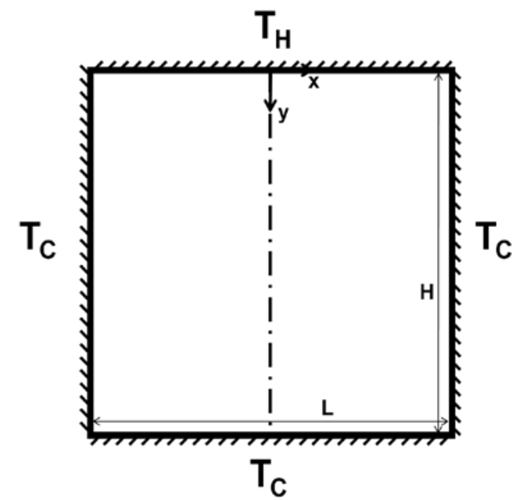
$$\mu_n=\cos\theta_n$$

$$\eta_{n,m}=\sin\theta_n\cos\varphi_m$$

$$t^*=t/\tau$$

$$x^*=x/L$$

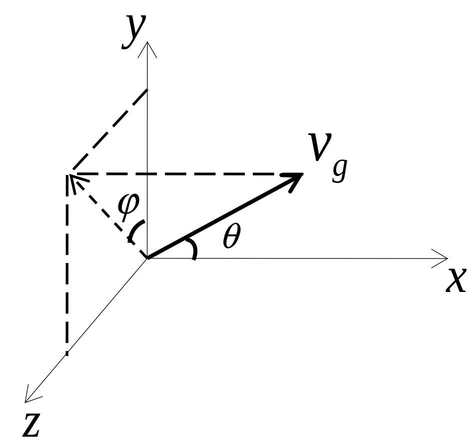
$$y^*=y/\mathrm{H}$$



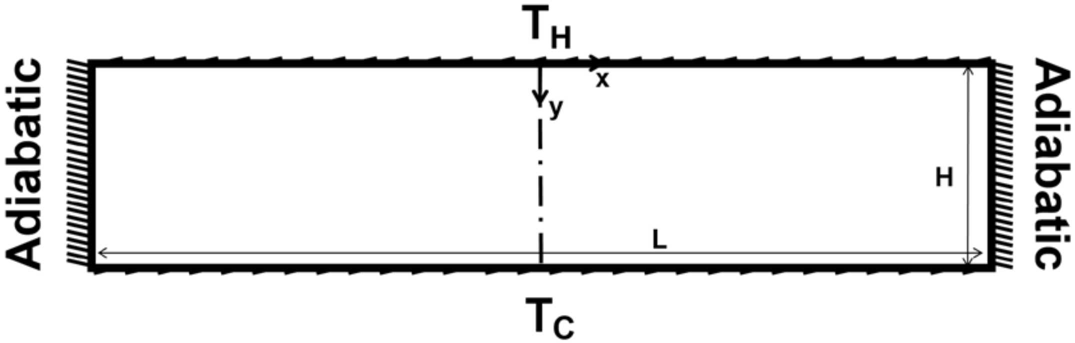
Discrete Ordinate Method (DOM)

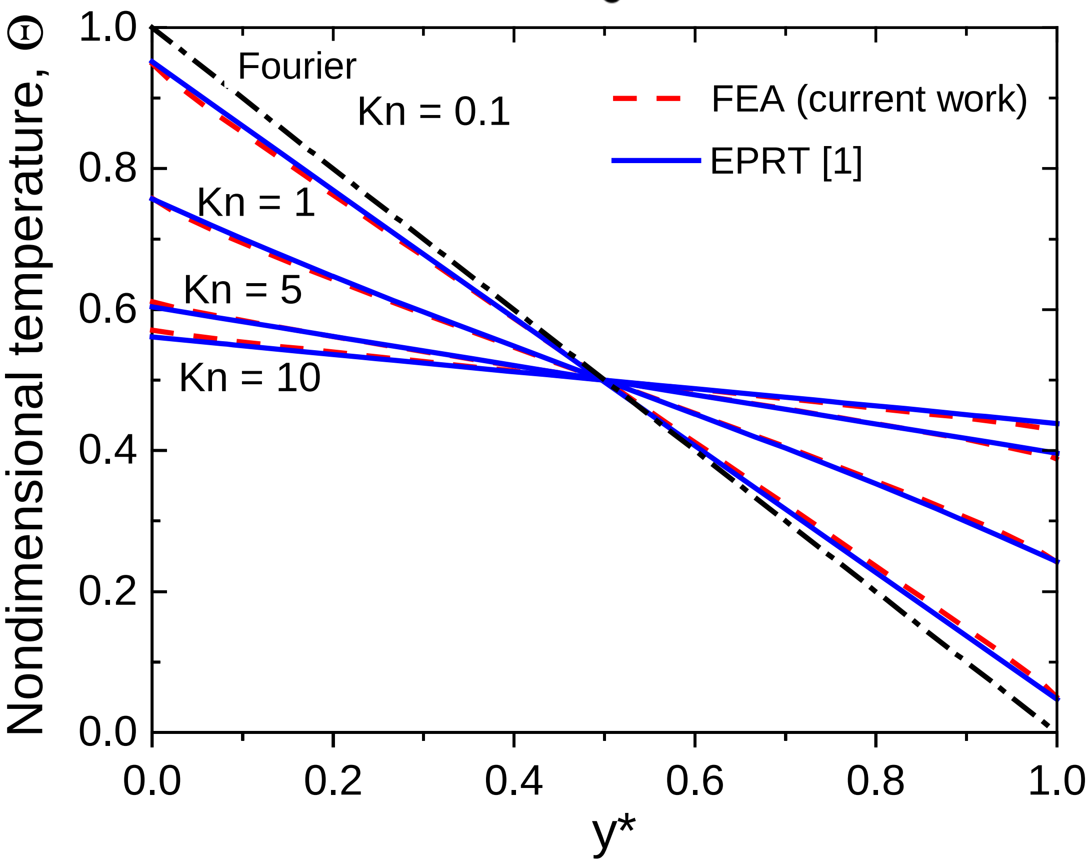
$$e''_0(\mathbf{r},t)=\frac{1}{4\pi}\int_{4\pi}e''(\mathbf{r},\hat{\mathbf{s}},t)\,d\Omega$$

$$\Rightarrow\quad e''_0(t^*,x^*,y^*)=\frac{2}{4\pi}\sum_n\sum_m e''_{n,m}(t^*,x^*,y^*)w_n w'_m$$



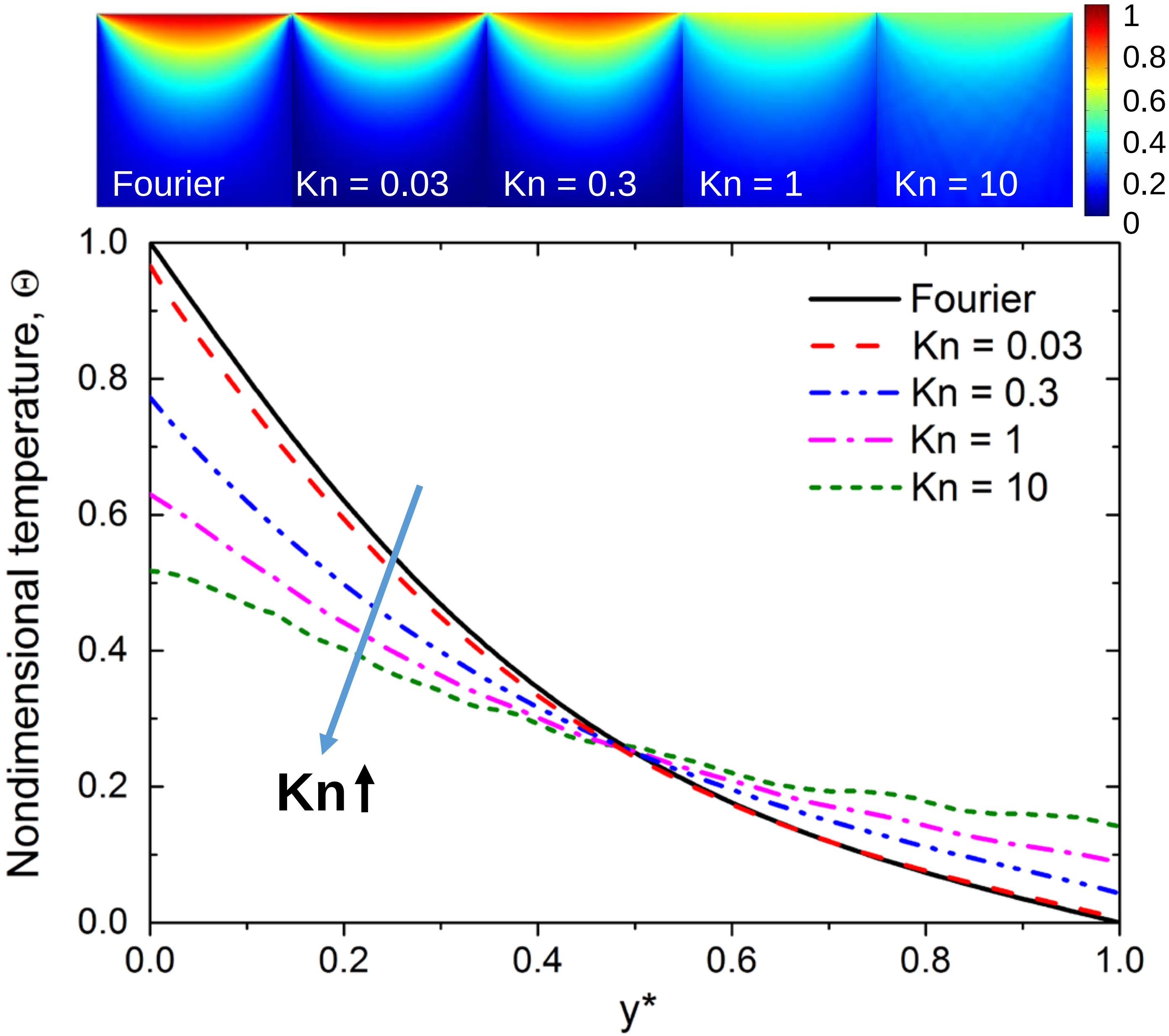
Validation (1-D thin film)



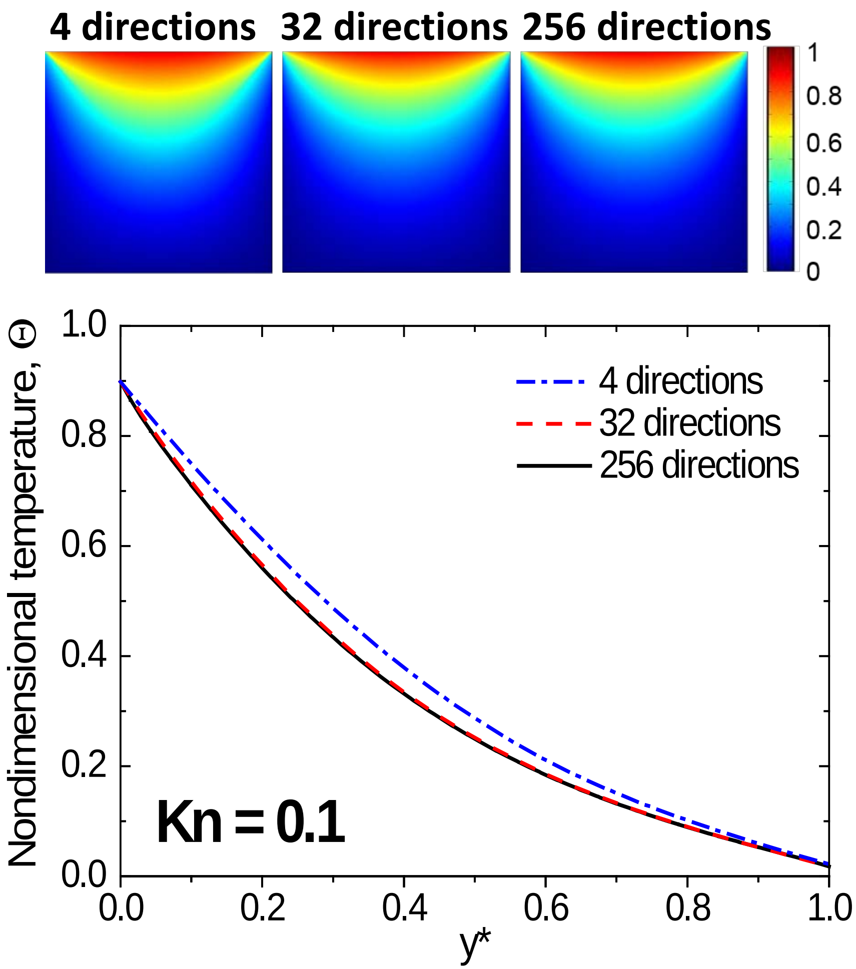


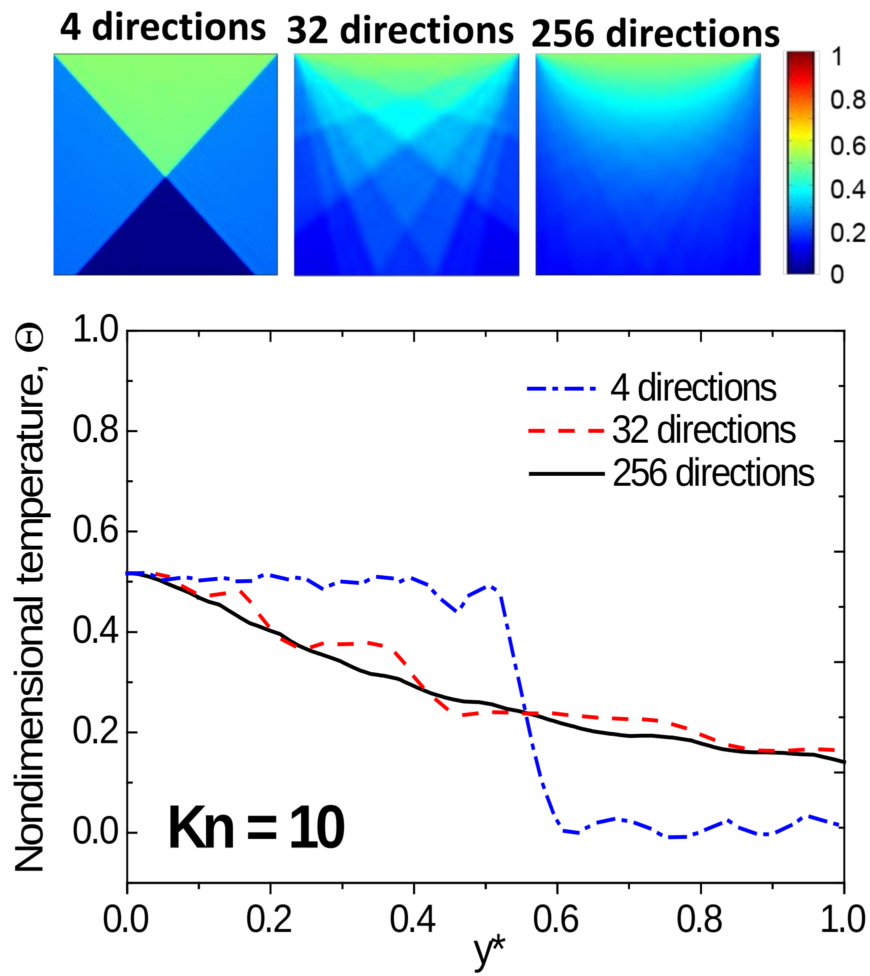
[1] G. Chen, Nanoscale Energy Transport and Conversion,Oxford University Press, 2005.

Results


Fourier
Kn = 0.03
Kn = 0.3
Kn = 1
Kn = 10
1
0.8
0.6
0.4
0.2
0
Nondimensional temperature, Θ
1.0
0.8
0.6
0.4
0.2
0.0
Fourier
Kn = 0.03
Kn = 0.3
Kn = 1
Kn = 10
Kn↑
0.0
0.2
0.4
0.6
0.8
1.0
y*

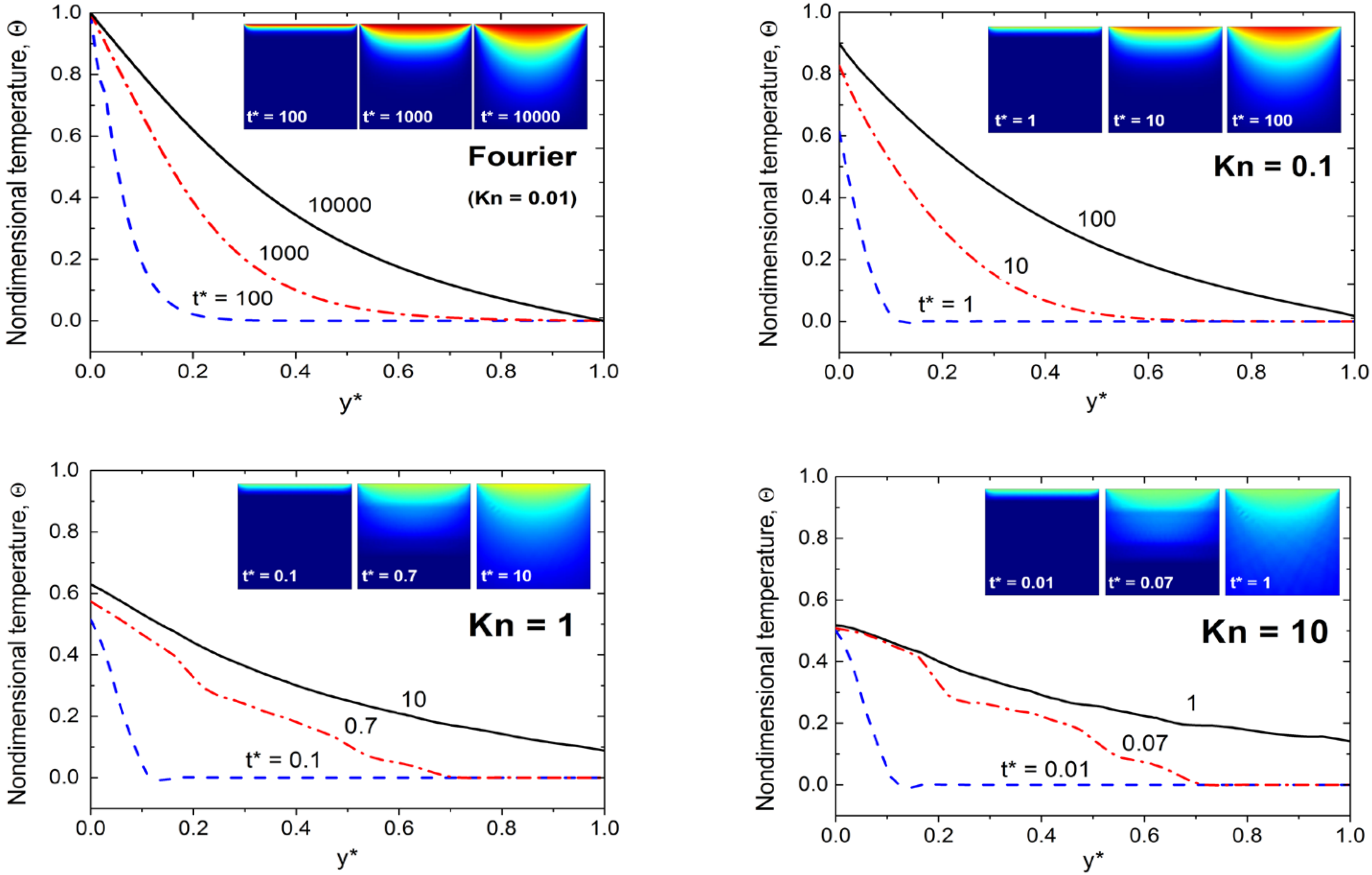
Ray effect





Diffusive

Transient solution



$$10\tau / \text{Kn}$$

Conclusion

- COMSOL can calculate sub-continuum phonon heat transport.
- FEA-DOM combination is used in COMSOL for ballistic-diffusive heat transfer.
- Modeling nanoscale heat transfer is easily accessible.

Acknowledgement

This work was supported by the National Research Foundation Grant funded by the Korean Government (NRF-2011-220-D00014) and the National Science Foundation (CBET-1067441). SH and KP also acknowledge the startup support at the University of Utah, including the computation at the Center for High-Performance Computing (CHPC).

Recently accepted in: International Journal of Heat and Mass Transfer

Doi: 10.1016/j.ijheatmasstransfer.2014.09.073

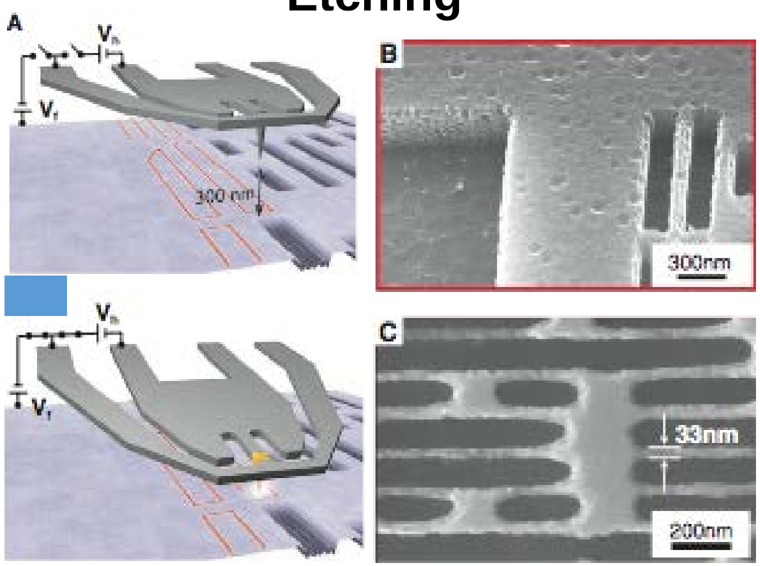

Thanks..

Introduction

Application:

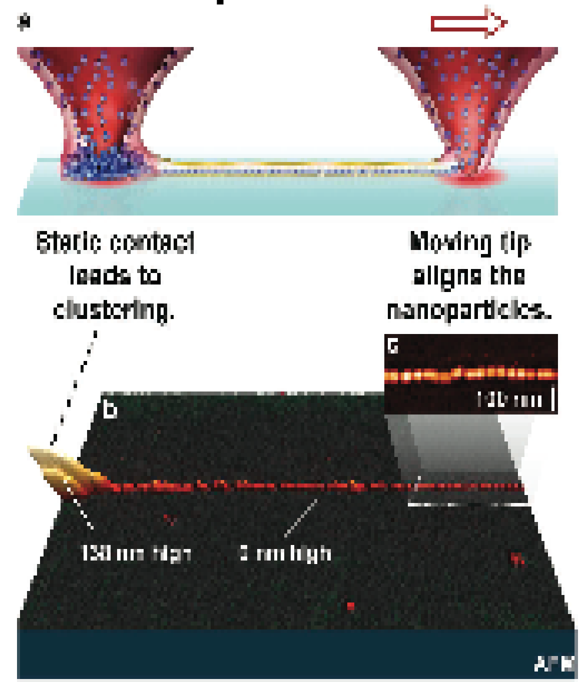
Thermomechanical data writing/reading
Thermal performance of extremely miniaturized electronic devices
Thermal etching
Thermal deposition

Etching



Pires et al., *Science*., **328** (2010)

Deposition



Lee et al., *Nano Lett*., **10** (2010)

Heat transfer equations

- Fourier equation

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$$

Energy conservation + Fourier's heat flux approximation

Used for heat conduction simulation for the last 2 centuries

Heat carriers travel with an infinite speed

Hyperbolic wave equation $\frac{1}{C^2}\frac{\partial^2 u}{\partial t^2} = \nabla^2 u$

- Hyperbolic heat equation (Cattaneo equation)

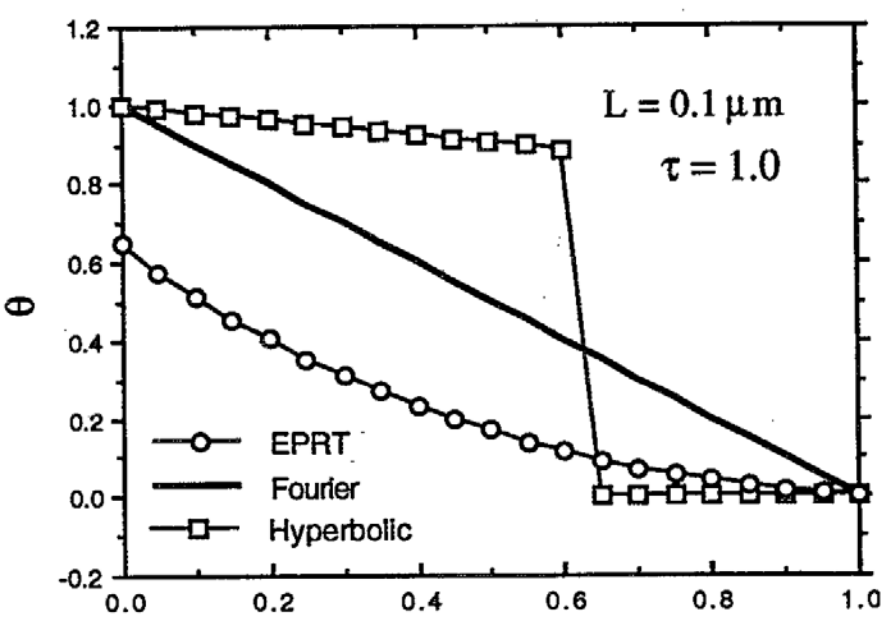
$$\tau \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \alpha \nabla^2 T$$

Finite speed of heat carriers $C^2 = \alpha / \tau$

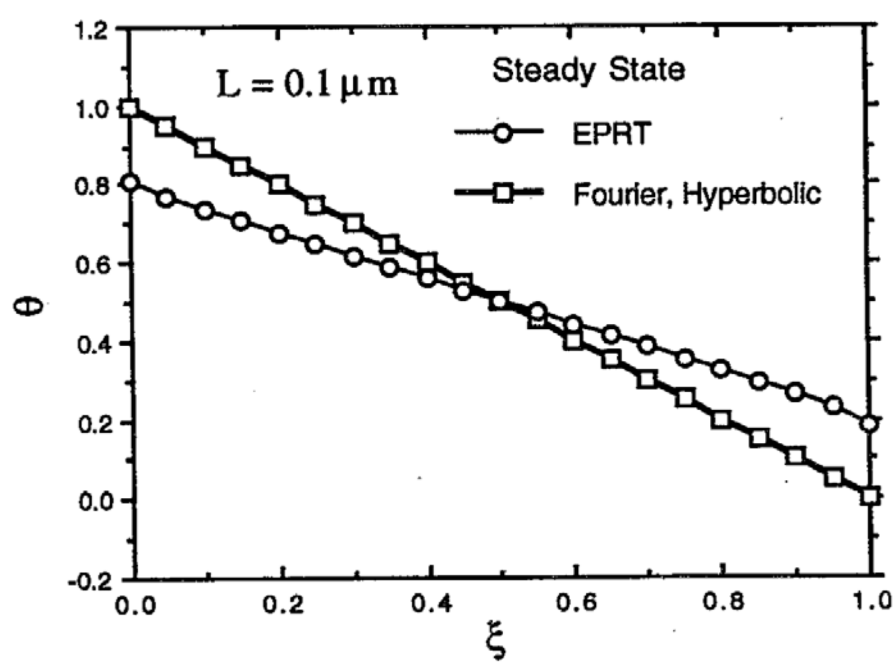
Good for short time scales but not for short spatial scale

Fourier and hyperbolic heat equations

Joshi and Majumdar, Journal of Applied Physics, 1993



Transient Fourier and Hyperbolic heat equation



Steady state Fourier and Hyperbolic heat equation

Boltzmann Transport Equation (BTE)

- Boltzmann transport equation (BTE)

BTE has a statistical base based on energy carriers distribution

$$\frac{\partial f}{\partial t} + \mathbf{v}_g \cdot \nabla f = \left[\frac{\partial f}{\partial t}\right]_{scattering}$$

f frequency dependent distribution function

$\mathbf{v}_g$ group velocity of energy carriers (phonons)

- Relaxation time approximation

$$\left[\frac{\partial f}{\partial t}\right]_{scattering} = \frac{f_0 - f}{\tau}$$

f_0 equilibrium Bose-Einstein distribution

τ effective relaxation time

Eqs

$$e_0''(t^*, x^*, y^*) = \frac{2}{4\pi} \sum_n \sum_m e_{n,m}''(t^*, x^*, y^*) w_n w_m'$$

$$\sum_n \sum_m w_n w_m' = 2\pi$$

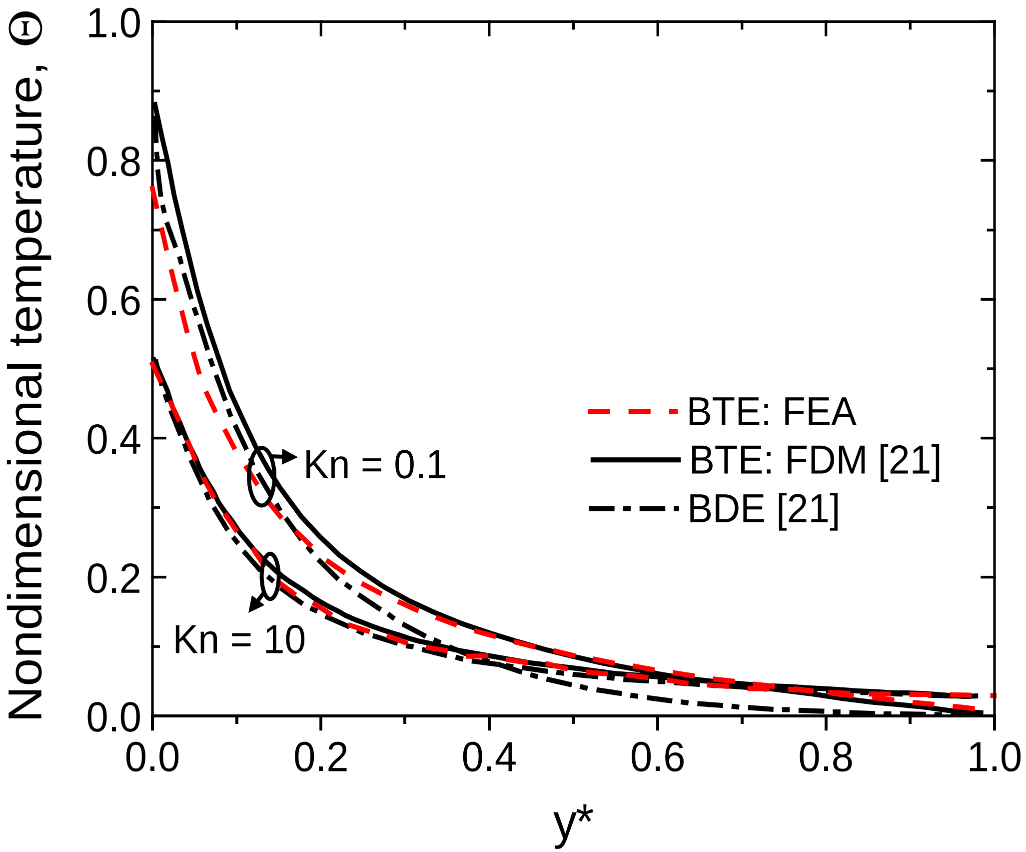
$$T(t^*, x^*, y^*) = \frac{4\pi e_0''(t^*, x^*, y^*)}{C} = \frac{2}{C} \sum_n \sum_m e_{n,m}''(t^*, x^*, y^*) w_n w_m'$$

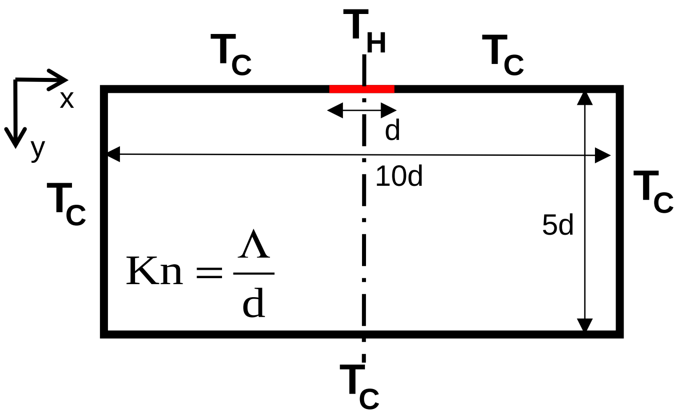
$$q_x''(t^*, x^*, y^*) = 2v_g \sum_n \sum_m e_{n,m}''(t^*, x^*, y^*) \mu_n w_n w_m'$$

$$q_y''(t^*, x^*, y^*) = 2v_g \sum_n \sum_m e_{n,m}''(t^*, x^*, y^*) \eta_{n,m} w_n w_m'$$

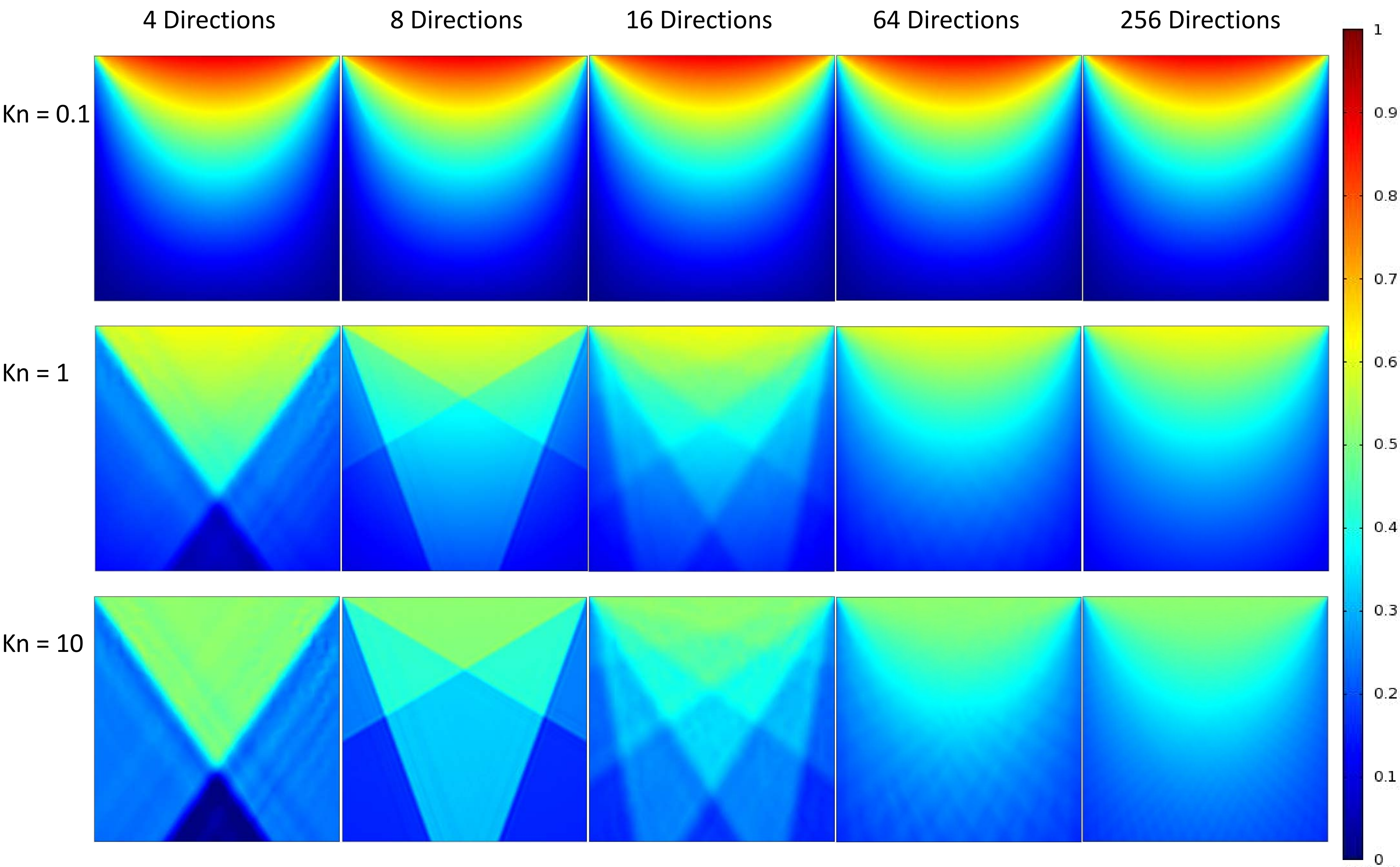
$$e''(\mathbf{r}_b, \mathbf{s}) = e_0''(\mathbf{r}_b) = \frac{CT_b}{4\pi}$$

COMSOL model





Ray effect



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COMSOL model