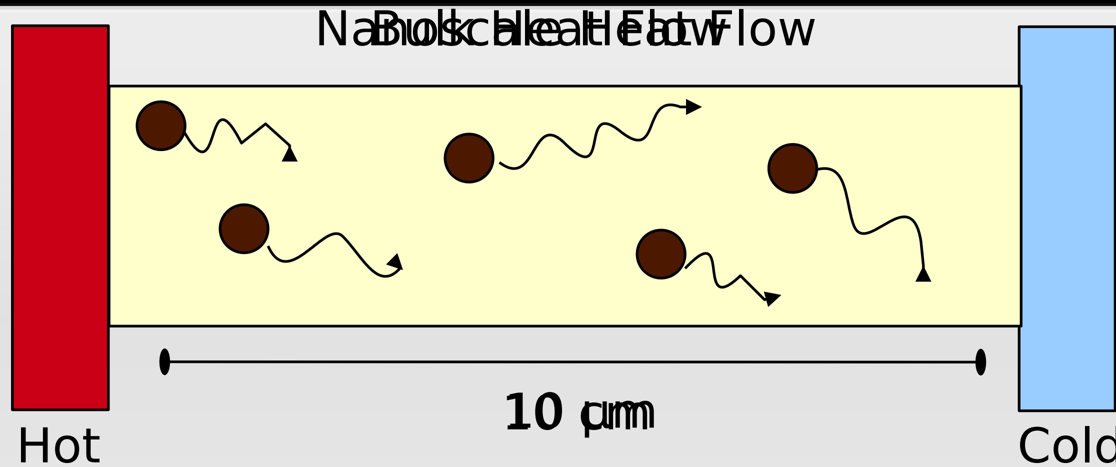
Presented at the COMSOL Conference 2008 Boston

Turning Up the Heat: Modeling Nanoscale Heat Flow

Sarah Palaich and Brian Daly
Department of Physics and Astronomy
Vassar College
Poughkeepsie, NY

COMSOL Conference 2008
Boston, MA

What is Nanoscale Heat Flow?



- Bulk heat flow well understood
- In semiconductors, phonons are the heat carriers
- Nanoscale, when the phonon mean free path (MFP) is equivalent to bulk dimensions

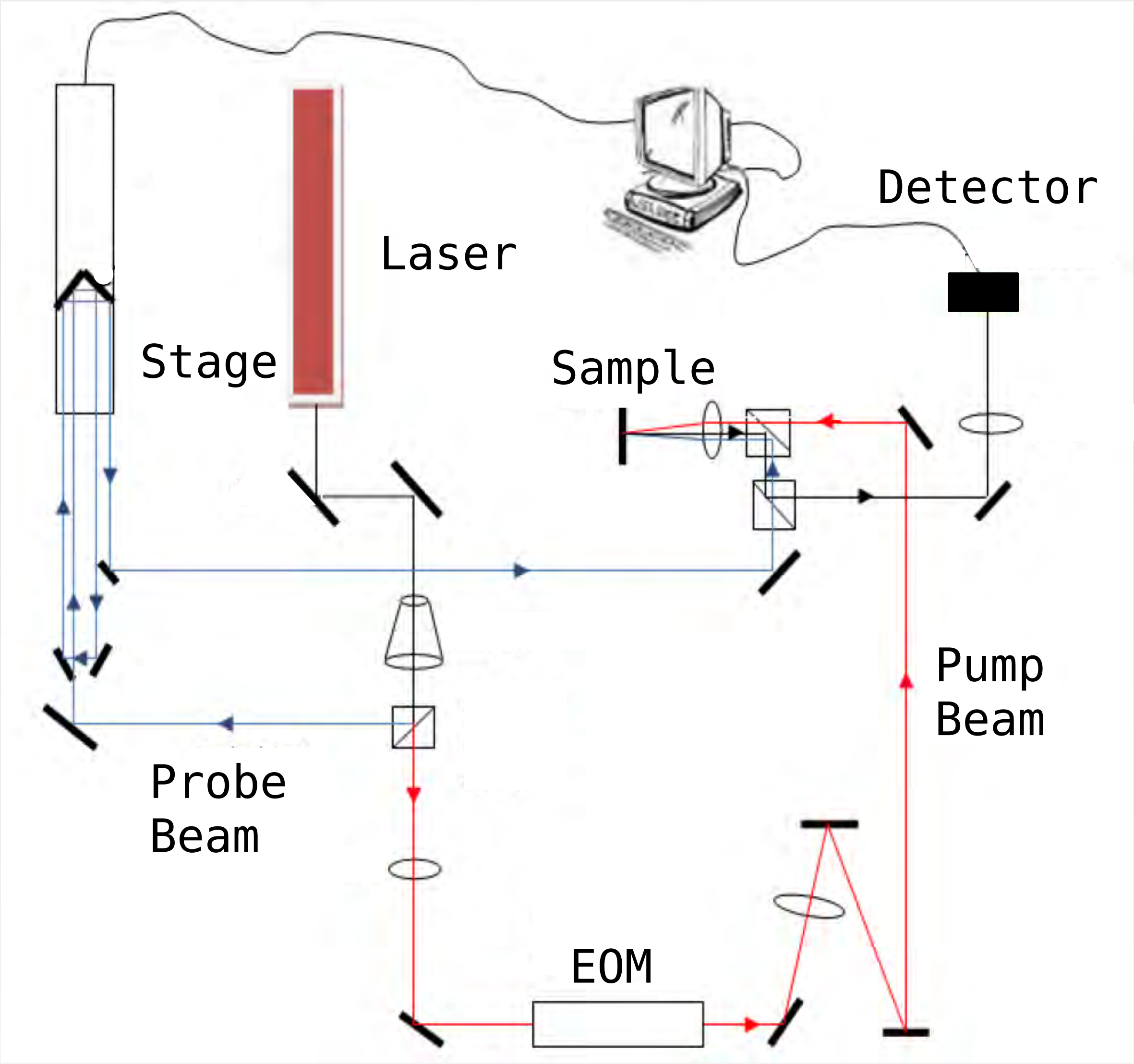
Why COMSOL Models?

- Nanotechnology necessitates a better understanding
- Thermal management in nm sized devices
  - Insulators
  - Semiconductors
- Boundaries play a significant role since phonon-boundary interactions important

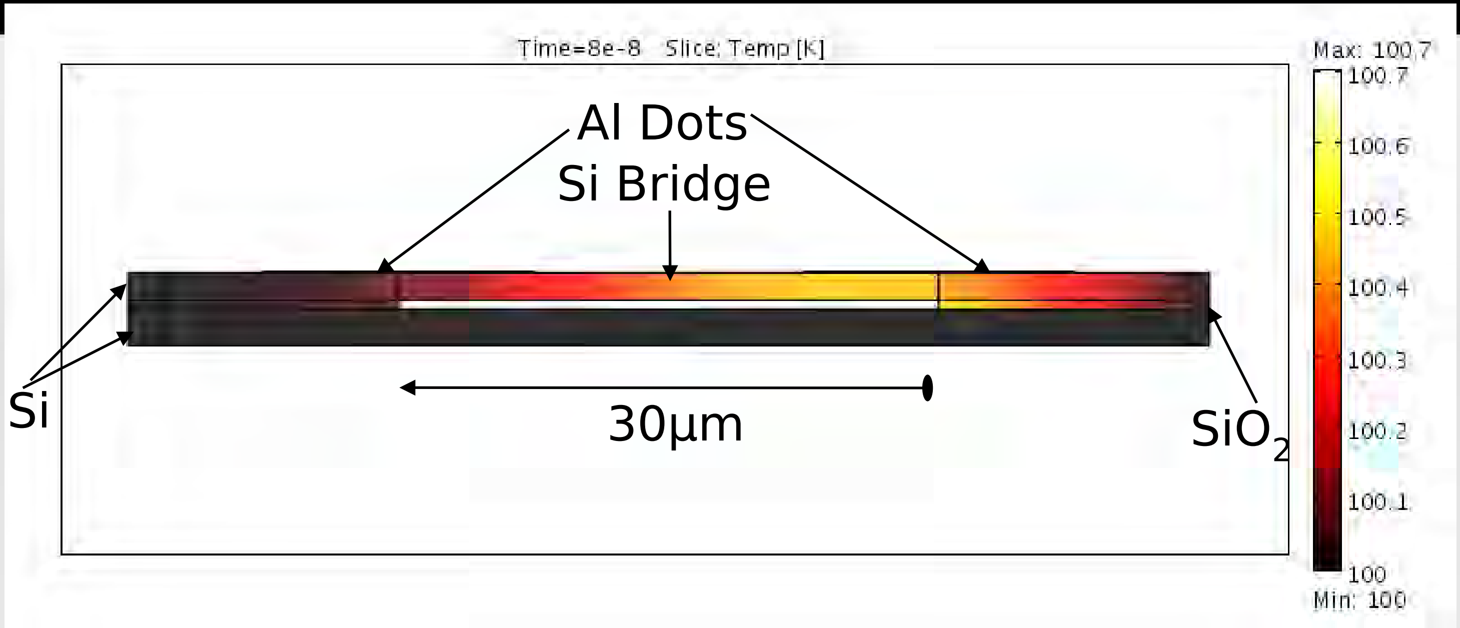
- COMSOL can simulate the theoretical models
- Use Heat Transfer Module as first step
- Use PDE mode to create custom heat flow model
- Eventually link bulk and nanoscale via COMSOL's boundary settings

Lab Applications

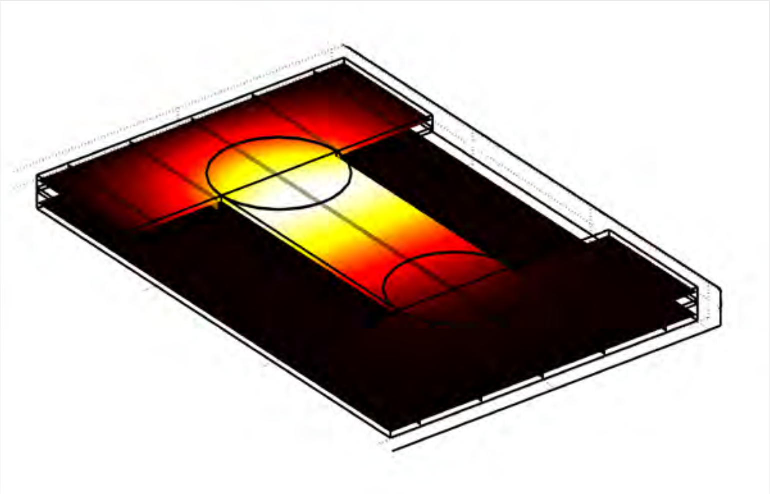
- Optical pump-probe experiment; time domain thermoreflectance
- Heats (pump) and measures temperature (probe) of thin films
- Ultrafast laser with picosecond pulses
- Time evolution of temperature measurements



COMSOL Lab Model

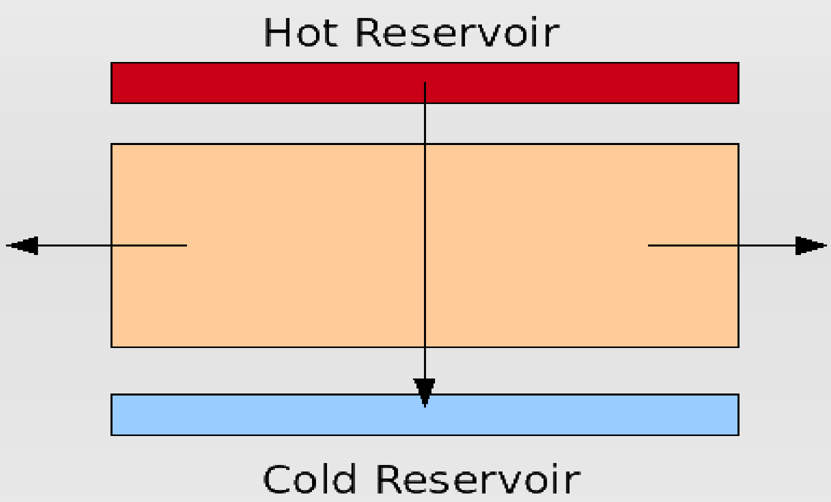


- Simulation at 100K
  - Increase of 10th degree, edge of detectability
- Created in General Heat Transfer Module (GHTM)
  - Bulk, not Nanoscale

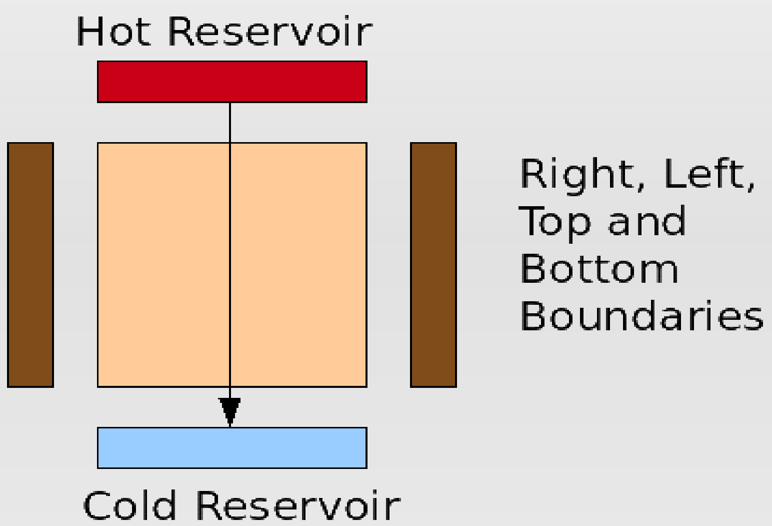


Nanoscale Geometries

- Thin Film



- Nanowire



- Thin Film: Flow from hot to cold reservoir across a distance that is comparable to the mean free path of the heat carriers, phonons in our models.
- Nanowire: The horizontal boundaries factor into the transfer of heat due to interactions with the heat carriers.

Theoretical Models of Heat Flow

- Boltzmann Transport Equation (BTE)
  - Phonon model interpreted in terms of the the BTE
    - Could provide an accurate nanoscale model
  - Calculates velocities and scattering rates for all phonon frequencies
- Cumbersome
  - Difficult to model complex geometries
  - Boundary conditions are complicated
- Seek a PDE describing energy transport
- Nanoscale regime
  - Temperature comes into question since heat carriers do not reach stable equilibrium

Cattaneo and Fourier Equations

- Fourier Equation

  $$\frac{\partial u}{\partial t} = \nabla\left(\frac{\kappa}{c}\nabla u\right)$$

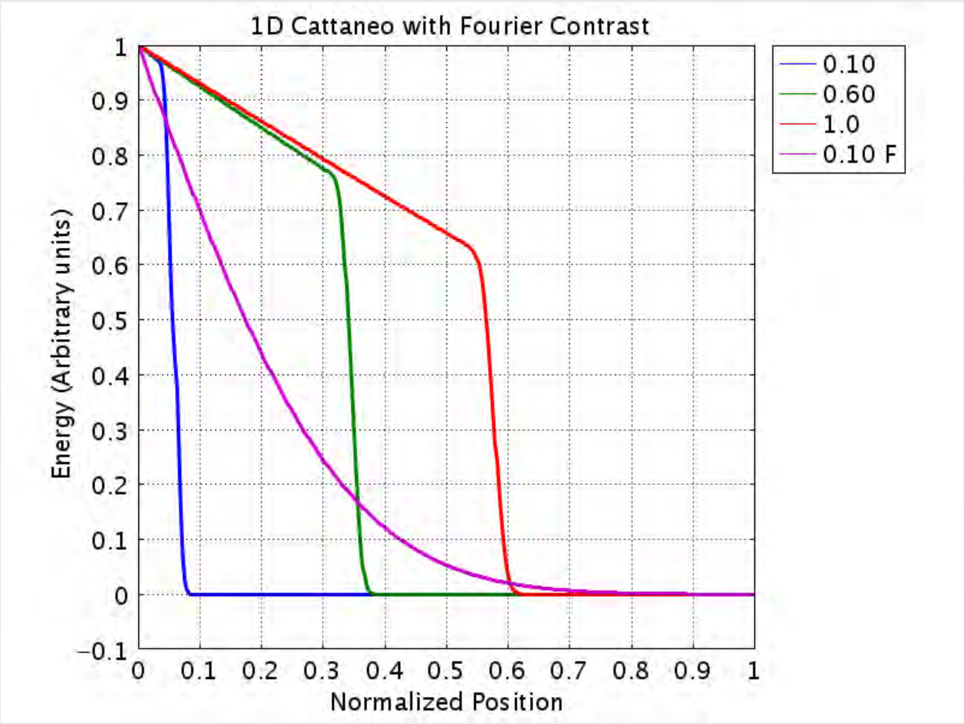
  - Basic partial differential equation
  - Describes bulk heat transport
  - Inaccurate at short nanoscale times since it allows instantaneous heat flow

- Cattaneo Equation

  $$\tau\frac{\partial^2 u}{\partial t^2} + \frac{\partial u}{\partial t} = \nabla\left(\frac{\kappa}{c}\nabla u\right)$$

  - Adds second order time derivative
  - Restricts speed of heat transport due to finite velocity of heat carriers, phonons
  - Accurate for bulk heat flow at short times

Cattaneo in COMSOL



1D COMSOL Solution to the Cattaneo Equation at three times and Fourier Equation at one time.

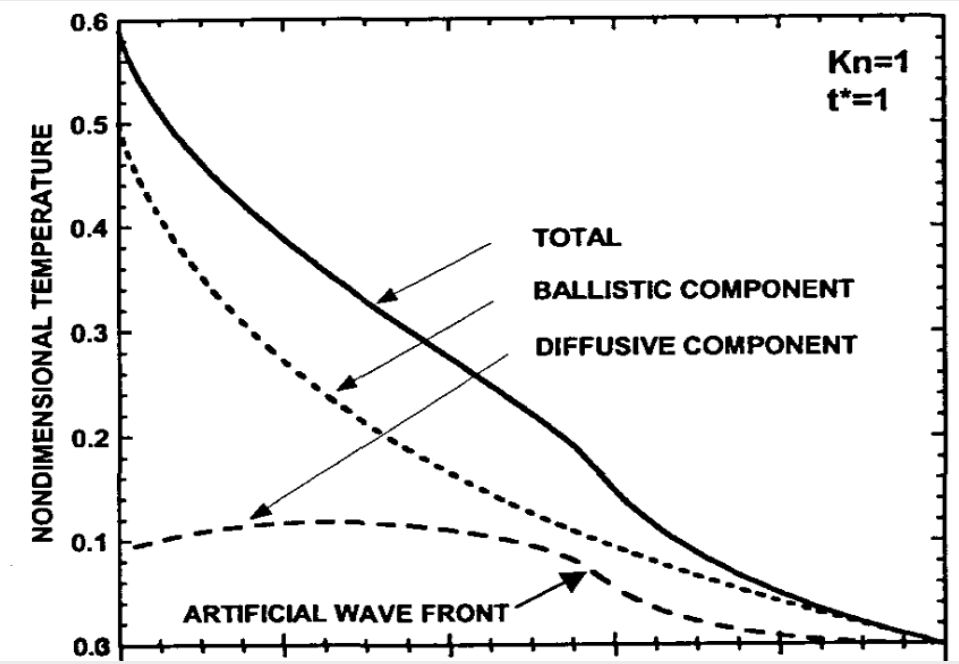
- 1D COMSOL model using General PDE Mode
- Accurate match to analytical solution to Cattaneo Equation
- Steep drop due to finite speed of heat carriers
- Stark contrast at early times to regular Fourier Equation

Radiative Boundary Heat Flow

- Chen posited Ballistic-Diffusive Equations (BDEs)

$$\tau C\frac{\partial^2 u_m}{\partial t^2}+C\frac{\partial u_m}{\partial t}=\nabla \boxed{\kappa}\nabla u_m \boxed{-}\nabla\cdot \boldsymbol{q}_b$$

  - Heat flux term $\mathbf{q_b}$
- Introduces Ballistic or Radiative Boundary Conditions as a source term for the Cattaneo Equation

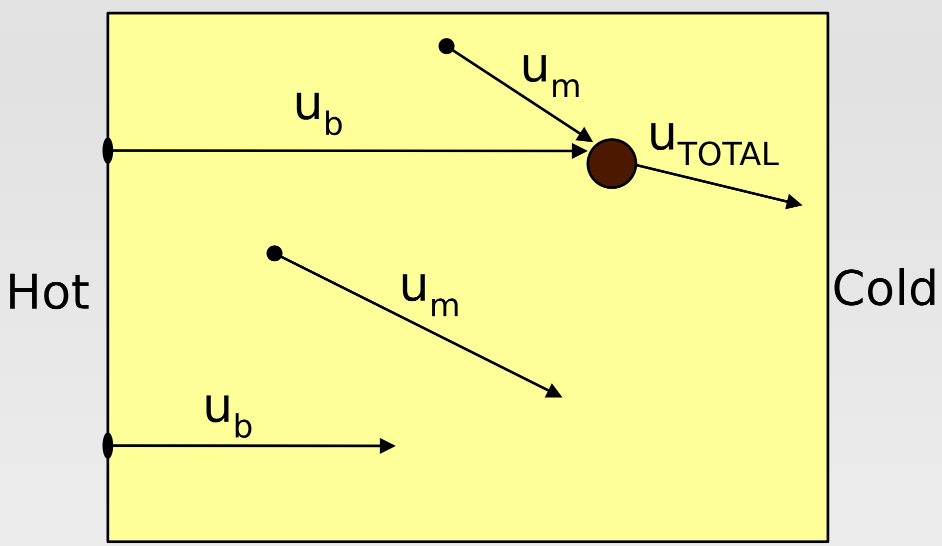


Chen's solution to his BDE with non-dimensional energy and distance

G. Chen, Ballistic-Diffusive Equations for Transient Heat Conduction From Nano to Macroscales, *J. of Heat Transfer*, **124**, pp. 320-328 (2002)

Heat Flux from Boundaries

Boundary and Medium Components



$u_{TOTAL} = u_b + u_m$

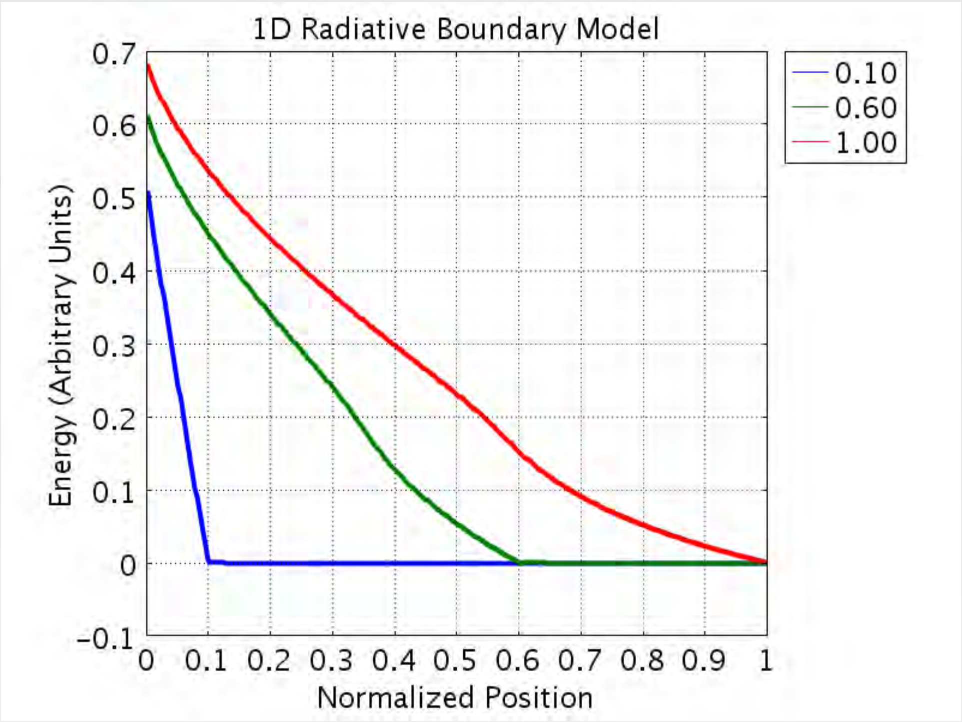
- Ballistic Flux Term Orginates from Boundary

$$q_b(\eta, t_{NORM}) = \frac{1}{2}\int \mu e^{-\frac{\eta}{\mu\xi}} d\mu$$

$$t_{NORM} = \frac{t}{\tau} \quad \mu_t = \frac{x}{vt} \quad \eta = \frac{x}{L} \quad \xi = \frac{\Lambda}{L} \quad 0 \le \mu_t \le 1$$

- Eliminates Thermal Contact (Reservoirs)
- Flux term is both:
  - u component from the boundaries
  - source term for the PDE governing u in the medium

Radiative Boundaries in COMSOL

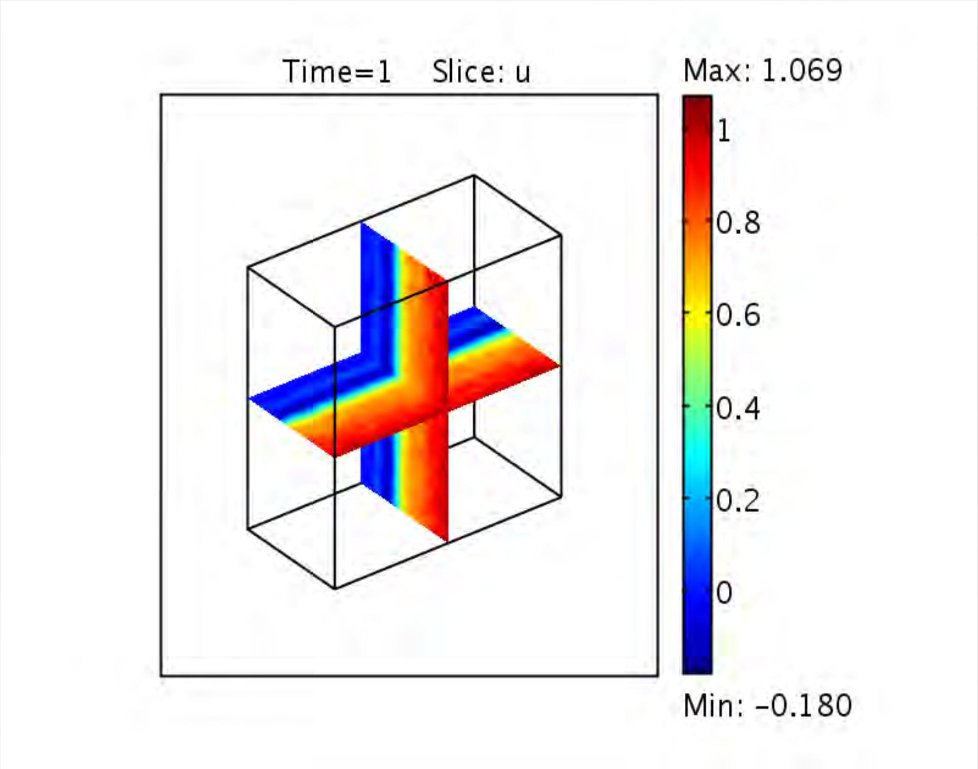


1D COMSOL solution with radiative boundaries.

- Using PDE Mode with Cattaneo Equation in the Subdomain settings
- Uses a series approximation for the heat flux term
- General trend matches Chen's results
- Evidence of the Cattaneo cliff is visible in the kinks at t = 0.6 and 0.3

Future Modeling

- Improve boundary conditions
- Move to 3D models
  - Thin Film
  - Nanowire
- Simulation of Experiment
  - Material Properties
  - Interface between nanoscale and bulk



3D COMSOL Solution to the Cattaneo Equation at one time. The light blue line is the cliff seen the 1D Cattaneo.