Characterizing Errors and Uncertainties in NEMD Simulations of Phonon Transport

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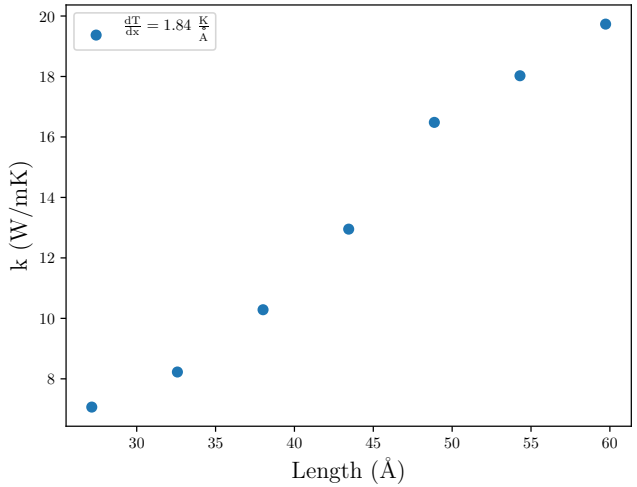
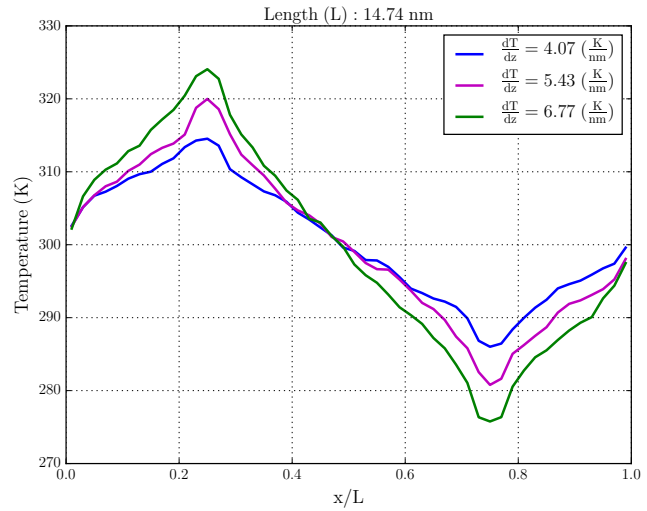
NON-EQUILIBRIUM MD

- Widely used to study thermal (phonon) transport in non-metallic systems (C,Si,Ge).
- System subjected to a temperature gradient using thermostats.
- Steady-state thermal energy exchange between the thermostats is used in Fourier's law to estimate bulk thermal conductivity (κ).
- Estimates are uncertain and severely under-predicted.
  - Simulation length-scales $\ll$ phonon mean free path.
  - Thermostats reduce correlation b/w vibration modes.

SOURCES OF UNCERTAINTY

- Bulk thermal conductivity is size-dependent.
- Variability in applied thermal gradient (Kapitza effect).
- Choice of the inter-atomic potential.
- Nominal estimates of the potential parameters.



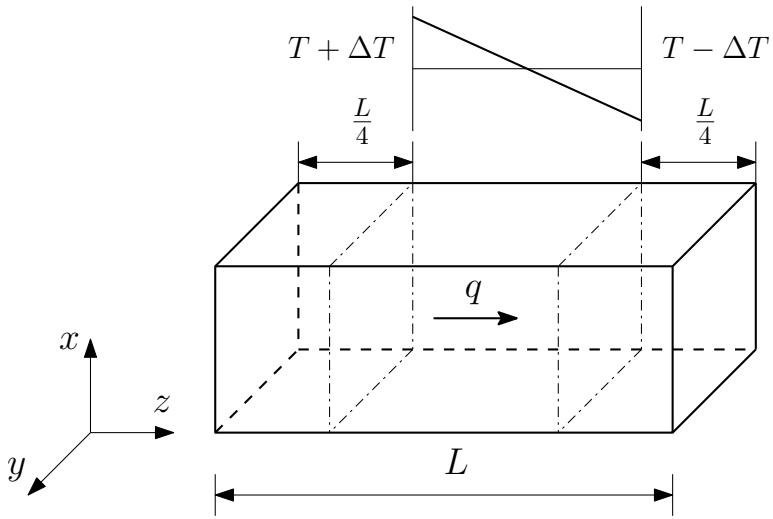


SPECIFIC RESEARCH GOALS

- Quantify discrepancy in κ between predictions and data.
  - Construct a response surface for $\kappa(s, \frac{d\theta}{dx})$.
- Perform sensitivity analysis of the potential parameters.
  - Estimate derivative-based sensitivity measures (DGSM).
- Construct a reduced order surrogate for κ using sparse NEMD predictions.
  - Use the surrogate for forward propagation of uncertainty, and global sensitivity analysis.
- Calibrate the *important* parameters in a Bayesian setting.

PROBLEM SET-UP

Lattice Constant, a (Å)	5.43
Width, Height (Å)	$22a$
Δt (ps)	0.0005
Boundary Condition	Periodic
Lattice Structure	Diamond
Inter-atomic Potential	Stillinger-Weber



PROBLEM SET-UP

- STAGES:

NVT $\rightarrow$ NVE $\rightarrow$ NVE

[Eqilibrate system to 300 K] [Equilibrate thermostats] [Generate Data]

N: Number of Atoms V: Volume T: Temperature E: Energy

- OBSERVABLE: Avg. energy exchange b/w thermostats (q)
- QOI: Bulk thermal conductivity (κ)

$$\kappa = \frac{q}{\left|\frac{dT}{dx}\right|}$$

- Appropriate selection of width, height, and simulation-time was ensured.

RESPONSE SURFACE: DISCREPANCY

- PC representation of the discrepancy, ϵ_d:

$$\epsilon_d \approx \epsilon_d^{PCE} = \sum_{k \in \mathcal{I}} c_k(T)\Psi_k(\boldsymbol{\xi}(\boldsymbol{\theta}))$$