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Frontiers in
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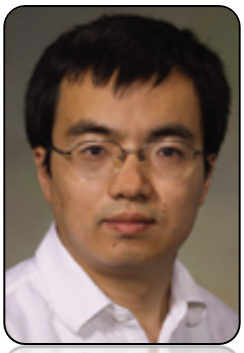
Lecture Series

Nanoscale Heat Conduction: From Molecular Dynamics to Nonlocal Models and Nonlocal Models to Local Models



Xiantao Li

Associate Professor, Department of Mathematics
The Pennsylvania State University

Friday, June 26, 2015
10 AM ◆ ISB2/Wanapum Room (155)

In addition to molecular dynamics modeling, Dr. Li's research interests include scientific computation, atomistic/continuum models of crystalline solids, and numerical solutions of differential equations. He focuses primarily on modeling of solids systems. He received his Ph.D. from the University of Wisconsin-Madison in 2002.

Heat conduction on nanoscale is known to exhibit non-Fourier behavior. Results from molecular dynamics simulations are readily available. However, they do not provide an efficient model for the transient process. In his talk, Dr. Li will present a mathematical derivation of a heat conduction model. The derivation begins with full classical molecular dynamics, leading to a nonlocal model—both in space and time. He also will discuss how to further simplify the nonlocal model by introducing additional equations for the heat flux, particularly by deriving a hierarchy of heat conduction models. The first few models in the hierarchy coincide with the traditional heat equation, the Cattaneo-Vernotte heat conduction model, and the Guyer-Krumhansl model. Yet, other models in the hierarchy are new. The accuracy of the new models will be demonstrated through a single-wall carbon nanotube and single-layer graphene.

Part of this talk is based on:

- X. Li, *Physical Review E*, 90 032112, 2014.
- X. Wu and X. Li, *Modelling and Simulation in Materials Science and Engineering*, 23, 015003, 2015.

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