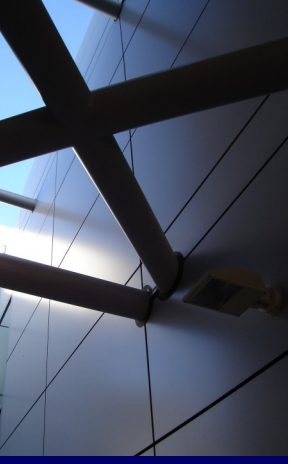

MECHANICAL ENGINEERING
DISSERTATION DEFENSE

The Department of Mechanical Engineering presents:

The Ph.D. Dissertation Defense of

Laura Rita de Sousa Oliveira

Thursday, April 13, 2017, 2-4PM
in Winston Chung Hall 205/206

Mixed Topics in Computational Thermal Transport

Doctor of Philosophy, Graduate Program in Mechanical Engineering
University of California, Riverside, April 2017
Dr. Alex P. Greaney, Chairperson

Heat transfer is ubiquitous in both naturally occurring and engineered materials. As technology progresses, the length- and time-scales of thermal transport decreases, becoming comparable with the mean free paths and relaxation times of the vibrations that drive it. Increasingly, an atomistic-level understanding of thermal transport is pivotal in predicting and controlling heat transport in materials and devices. Modeling approaches that permit an atomistic understanding of heat transport, and the implementation of complex approximations of the phonon Boltzmann transport formalism include classical molecular dynamics and density functional theory (DFT). Results are presented for equilibrium molecular dynamics (EMD) simulations of the thermal conductivity of a series of clustering and non-clustering point defects in graphite using the Green–Kubo method, aimed to advance our knowledge of the evolution of the microstructure of graphite while in service in a graphite-moderated nuclear reactor. The Green-Kubo method — commonly used for predicting transport properties by scientists and engineers across fields — relates the property of interest to the lifetime of fluctuations in its thermodynamic driving potential. The integral of the autocorrelation fluctuations requires a long averaging time to reduce remnant noise and is a principal source of error. A new approach is proposed to quantify ¬— on-the-fly — the uncertainty on transport properties computed using the Green-Kubo formulation, based on recognizing that the integrated noise is a random walk. EMD is also used to explore thermal transport in breathing metal¬–organic frameworks (MOFs), coveted for numerous applications due to their large surface area and modularity. A simple geometric model of thermal conductivity is proposed as a heuristic for the quick evaluation of transport in flexible MOFs, and a quantum-based approach is undertaken to explore deviations from the heuristic, such as rattler modes and phonon-focusing. Phonon properties calculated with DFT for (1) uranium dioxide and (2) silicon, for fuel and spintronics applications respectively, are also briefly discussed.