Abstract
Research and development of mechanical components with moving interfaces requires being able to predict how operating conditions will affect the interfacial materials. This is typically done using empirical formulae fit to experimental data. Although extensive experimental studies have enabled highly accurate parameters for these models, they are limited in that, for each interface to be studied, more experiments must be performed. Further, most empirical models cannot be used for design of previously undefined materials. An approach to addressing this issue is interface characterization using physics-based simulations. One example, and the focus on this talk, is molecular dynamics simulation – a computational “experiment” where an atomic-scale system is defined, allowed to evolve according to Newton’s second law, and then observations are made based on its evolution. Once validated, this model becomes a powerful predictive tool for cases where no experimental data is available. Perhaps more significantly, the flexibility of molecular dynamics for modifying atomic structure may enable application-specific interface design.

This talk will focus on two illustrations of molecular dynamics simulation as a tool for interface characterization: confined fluid compressibility and atomic stick-slip friction. First, simulations are used to study the compressibility of three model lubricants under varying degrees of confinement and subject to a range of loads. The simulation-predicted densities are compared to those of an empirical, bulk fluid compressibility model and it is found that molecular dynamics simulation can predict bulk compressibility if the model film thickness is sufficiently large relative to the characteristic length scale of the fluid molecule. These simulations also lend new insight into how the molecular structure of a fluid affects its compressibility. The second interface characteristic that will be discussed is atomic stick-slip. Atomic stick-slip occurs when sliding does not occur stably; instead, two surfaces stick together and lateral strain builds up, at some critical point the surfaces slide (usually by one atomic lattice site), and then they lock together again. This phenomenon is important in itself because of the need to control energy dissipation associated with an abrupt slip. However, it is also an example of a so-called infrequent event system in which time can be separated into the short scale of a “transition” event and the long scale of the periods between transition events. Modeling an infrequent event system enables use of accelerated molecular dynamics techniques that overcome the time-scale limitation introduced by necessarily short simulation time steps. One such method, parallel-replica dynamics, and its application to atomic stick-slip friction will be discussed.

The high-level goal of this talk is to communicate the potential for an engineering approach where physics-based simulations resolve mechanisms validated by experiments, experimental phenomena are explained by reference to the models, and together they form the basis for a new comprehensive approach to interface design.

Bio:
Ashlie Martini is an Assistant Professor of Mechanical Engineering at Purdue University. She received her Ph.D. in Mechanical Engineering from Northwestern University in 2007.