

Amgen Seminar Series in Chemical Engineering
in
Cherry Auditorium, Kirk Hall, 1 PM

Presents on March 31, 2016

**The Lattice Kinetic Monte Carlo Method as a Versatile Tool for
Simulating Diverse Micro and Mesoscale Phenomena**

By

Dr. Talid Sinno
Department of Chemical and Biomolecular Engineering
University of Pennsylvania

Lattice-based, or 'on-lattice', kinetic Monte Carlo simulations are attractive because of their relative computational simplicity and efficiency, and have been employed to simulate an enormous range of non-equilibrium physical, chemical and biological phenomena. In a kinetic Monte Carlo simulation (also referred to as dynamic Monte Carlo or the Gillespie method), which is typically applied to a collection of discrete particles, rates must first be specified for a set of 'events', such as a hop of an atom from one lattice site to another or a reaction between two particles. The universe of events and the associated rates are input to the kinetic Monte Carlo simulation, and must be obtained by some other means. The simulation is then carried out by executing events in a biased stochastic sequence.

In this talk, variants of the lattice kinetic Monte Carlo method are applied to several distinct situations, ranging from microstructure evolution in semiconductor crystals, to cellular aggregate formation in blood flow, to coarse-grained simulations of phase evolution in generalized liquid-vapor systems. These diverse examples are used to illustrate the simplicity and flexibility of the general lattice kinetic Monte Carlo framework as a powerful computational tool, but also the potential pitfalls related to its application in certain situations. In this regard, special emphasis is placed on the discussion of (1) reduced degree-of-freedom representations (via coarse-graining) and the concomitant loss of entropy, and (2) simulation of systems of particles subject to external advective fields such as fluid flow.

This series at the University of Rhode Island is made possible through the
generosity of Amgen, West Greenwich, R.I.

Refreshments provided by the Joseph Estrin Endowment.