**TEMPLE UNIVERSITY**
Department of Mathematics

# Applied Mathematics and Scientific Computing Seminar

Room 617 Wachman Hall

Wednesday, 28 November 2018, 4:00 p.m.

## Approaches to Metastability in Materials Science

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**Abstract.** One of the outstanding challenges in atomistic simulations of materials is how to reach physically meaningful time scales. While the fundamental time scale of the atomistic models is that of the femtosecond, physically meaningful phenomena may take microseconds or longer to occur. This precludes a direct numerical simulation with, for instance, a Langevin model of the material from reaching physical time scales. The time scale separation challenge has motivated the development of a variety of multiscale methods, including accelerated molecular dynamics, kinetic Monte Carlo, phase field models, and diffusive molecular dynamics. In this talk, I will survey some of these approaches and discuss common mathematical assumptions that underlie them while also highlighting where approximations have been made. Rigorous results will be presented, where available, along with outstanding mathematical challenges.