

Joint Condensed Matter and Center for Soft Matter and Biological Physics Seminar Prof. James McClure

Research Computing, Virginia Tech

"Modeling multiphase flow and anomalous diffusion

with mesoscopic methods"

Monday, November 16, 2020

4:00pm - 5:00pm

Virtual Meeting:

Zoom Link: https://virginiatech.zoom.us/j/86195436231

Lattice Boltzmann methods provide a practical bridge between molecular- and continuum-scale models, relying on quasi-molecular interaction rules to simulate physics at significantly larger length and time scales compared to what is accessible from molecular dynamics. This talk will review approaches to develop mesoscopic models using the lattice Boltzmann method, with applications to wetting and spreading on heterogenous surfaces, fluid flow in porous media, and diffusion in electrochemical cells. Using simulation data, we consider how time-and-space averaging can be applied to understand scale effects in heterogeneous systems, particularly for long-wavelength fluctuations in non-equilibrium systems. Consequences for symmetry-breaking are explored within this context.

