



Network for Computational Nanotechnology & c-PRIMED Seminar Series

Seminar Notice. 1:30PM Tuesday, October 18, 2016
Potter Building, Fu Room, #234

Phase-field modeling of microdomains evolution on giant unilamellar vesicles and rapid development within MOOSE framework

Dr. Wen Jiang, Idaho National Laboratory

We will discuss some recent work in the development of computational methods for solving phase-field models. **The first part of the seminar will focus on the development of phase-field approach for modeling the evolution of microdomains on giant unilamellar vesicles (GUVs).** A coupled chemo-mechanical model is developed to capture the formation and evolution of microdomains on the deforming surface of giant unilamellar vesicles (GUVs). The GUV is assumed to consist of a binary mixture of lipid species. The chemical energy is characterized by a Cahn–Hilliard type density functional that characterizes the line energy between domains of different species. The generalized Canham–Helfrich–Evans model provides a description of the mechanical energy of the vesicle membrane. This coupled model is cast in a diffuse-interface form using the phase-field framework. The resulting fourth-order non-linear system of equations is efficiently solved by an adaptive hierarchical refinement approach. We will present interesting results that demonstrate the effect of coupling between domain formation and vesicle shape changes.

The second part of the seminar will focus on the development of general phase-field models within Multiphysics Object Oriented Simulation Environment (MOOSE) framework. The MOOSE framework allows for rapid development of advanced phase field models. We will first revisit the phase-field model of the vesicle example and demonstrate how easy it is to implement within MOOSE framework. Furthermore, MOOSE framework provides a powerful tool for coupling the phase field model to other physics, such as heat conduction and deformation, and for determining bulk material properties as the microstructure evolves. The simulation results are used to develop and refine mechanistic materials models for macroscale modeling. We will present various numerical examples using MOOSE framework.

Dr. Wen Jiang is currently a postdoctoral researcher in the Fuel Modeling and Simulation Department at Idaho National Laboratory (INL). He received his Ph.D. in Mechanical Engineering and Materials Science from Duke University. Dr. Jiang has extensive experience in computational methods and materials modeling. His research focuses on developing of numerical methods that enable the investigation of emerging theories in applied mechanics and materials science, with a particular emphasis on the important role played by interfaces and defects. At INL, he is team member of MARMOT and BISON research group and develops mechanics capabilities in INL's MOOSE framework. He has been involved in multiple DOE-sponsored projects that range from meso-scale material modeling to engineering structure modeling.