We will present an introduction to multiscale modeling and numerical analysis at the atomistic, mesoscopic, and continuum scales including interatomic potentials, energy landscapes, defects, molecular dynamics, and coarse-graining. We will also present an introduction to the mathematical foundations and numerical analysis for the mechanical and electronic structure of 2D materials.

Prerequisites are undergraduate numerical analysis and partial differential equations. All introductory material on atomistic and continuum modeling will be covered in the course notes and lectures.