Liquid structure and shearing, inhomogeneous fluids: a molecular dynamics simulation approach

Benjamin Dalton (RMIT University)

Abstract. Molecular dynamics (MD) is a well-established computer simulation technique used to deterministically model physical systems from an atomic and molecular perspective. MD has many applications in physics, chemistry, molecular biology and nanoscale engineering. In this presentation we consider various simplified MD systems that illustrate the use of external fields and heat baths, and we describe a novel method for calculating the structure of a liquid. We then briefly consider how we can apply these methods to the study of shearing flow in strongly inhomogeneous fluids. It is currently unknown how to accurately describe flow in fluids that exhibit large density gradients over nanoscopic length scales. Such an accurate description represents an important unsolved problem in the field of nanofluidics. By developing simplified models we are able to probe the nanoscale density and shear-flow coupling in a way that is not possible with other nanofluidic systems.