Multiscale Simulation of Molecular Fluids

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Understanding fluid physics at nanometer scale is important for many applications including water purification, gas separations, energy storage, DNA sequencing, etc. Molecular scale phenomena such as finite size of the molecule compared to the pore/slit size, restricted translational and rotational motions, ballistic diffusion, etc. pose challenges to the classical continuum theory of fluids. To overcome the limitations of the classical theory, molecular approaches such as quantum techniques, molecular dynamics and Monte Carlo methods are popularly used. However, these approaches are limited to small length and short time scales. Here, we discuss the development of a quasi-continuum theory to predict the structure, dynamics, and transport of confined fluids. Quasi-continuum theory seamlessly integrates molecular scale physics into classical theory and we demonstrate the accuracy of the approach by considering several examples.