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Brownian Dynamics Simulation of Pressure Induced Pore-Transport through an Incommensurate Channel

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Cells and organelles use pores embedded in their protective membranes to facilitate the transport of materials (ions, molecules, proteins, etc.) between their lumen and the surrounding environment. In the case of passive transport, flow of homogeneous particles through a pore channel can be driven by a non-equilibrium pressure differential. Previous work has modeled this system using random walks in a discrete state space of positions along the channel length. We extend this model to the continuum using Brownian dynamics simulation and include the Frenkel-Kontorova model by factoring the pair-wise interaction between the flowing particles and a periodic potential associated with the channel. The interplay between the equilibrium spacing of the particles and the intrinsic period of the channel's potential wells can result in spontaneous formations of pairs of incommensurations in the particle distribution throughout the channel lattice. We characterize these incommensurations as heavy and light domain walls and investigate how their movement and interactions facilitate pressure induced channel flow.