MULSTICALE MODELLING OF LIQUIDS WITH MOLECULAR SPECIFICITY

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Separation between molecular and mesoscopic length and time scales poses a severe limit to molecular simulations of mesoscopic phenomena. To solve this problem we propose a hybrid technique which enables to dynamically couple a molecular dynamics (MD) domain with a fluctuating hydrodynamics (FH) description of the surrounding liquid based on the Landau theory (see figure). This multiphysics approach is designed to study processes driven by the interplay between the molecular interactions at a small (nanoscopic) region and the hydrodynamic response at larger spatio-temporal scales. Examples are ubiquitous, in microfluidics, slippage of fluid over surfaces, wetting, crystal growth from fluid phase, vibrational properties of proteins via sound interaction.

Bridging spatio-temporal scales is the main objective of multiscale modelling and one of the "hot-topics" of the simulation community. However, compared to gas and solid phase, the hybrid description of the liquid phase is less developed. The present model is the first to solve decisive features: it works with accurate molecular description (chemical specificity), it is thermodynamically consistent up to the level of fluctuations, and it transfers sound across the hybrid MD-FH interface. Due to its relevance we consider water as working solvent and solve the reflection of sound by a lipid monolayer in aqueous solvent (set up shown in the figure). *To appear in PRL, preprint available.*