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Coupling atomistic molecular dynamics and fluctuating hydrodynamics: shear and sound[1] RAFAEL DELGADO-BUSCALIONI, Universidad Autonoma de Madrid, GIANNI DE FABRITIIS, Universidad Pompeu Fabra, Barcelona — Bridging spatio-temporal scales is the main objective of multiscale modeling and one of the hot-topics in the simulation community. However, compared to gas and solid phase, hybrid schemes based on molecular-continuum domain decomposition of the liquid phase are relatively less developed. The present hybrid model (see PRL 97, 134501 and PRE 76, 036709) is the first to include several decisive features: the molecular domain is described with atomistic accuracy (chemical specificity), and it is embedded within a continuum fluid description based on the Landau-Lifshitz fluctuating hydrodynamics equations. The hybrid scheme is thermodynamically consistent (e.g. the MD domain is an open subsystem in agreement with the grand canonical ensemble) and fluctuations of mass, momentum and stress are seamlessly connected across the molecular-continuum interface. As the scheme is based on mass and momentum conservation, it enables to solve shear and sound waves traveling across both domains. Due to its relevance we consider water as working solvent. As a test case, we have studied the reflection of sound waves by a lipid monolayer (DMPC) immersed in aqueous solvent.

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