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Multiscale computation of wetting transitions on micro/nanoscale solid structures CARLOS COLOSQUI, Princeton University, MICHAIL KAVOUSANAKIS, ATHANASIOS PAPATHANASIOU, National Technical University of Athens, IOANNIS KEVREKIDIS, Princeton University — Modern microfabrication techniques allow the construction of solid surfaces with micro or nanoscale structure. The artificial micro/nanostructure, when properly designed, produces smart surfaces capable of exhibiting surperhydrophobic or superhydrophilic wetting properties in an addressable manner The design and control of transitions between superhydrophobic and superhydrophilic states using minimal external actuation (e.g. via electro-wetting, UV radiation, etc.) is an active research area with enormous impact in microfluidics and materials science. In this work, we demonstrate a computational methodology that allows microscopic or mesoscopic models to perform numerical continuation and stability analysis at macroscopic level. The method's ability to compute stable and unstable wetting states via accurate dynamic simulations is extremely valuable for the optimal engineering design of micro/nanostructures. The computational methodology is demonstrated by employing a novel lattice Boltzmann model that captures critical interfacial phenomena such as disjoining pressure and vapor adsorption at the solid-fluid surface.

Carlos Colosqui
Princeton University

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