Direct Numerical Simulation of Nanofilm Instability Driven by Liquid/Solid Interactions

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The nanoscale interaction between liquid and solid molecules underlies fundamental phenomena for systems involving liquids on surfaces. In addition to giving rise to the contact angle of drops, this interaction drives the spontaneous rupture of nanofilms. We study this process by means of direct simulation of the Navier-Stokes equations using the Volume of Fluid interface tracking method. Our numerical method simulates the liquid/solid interaction, and permits the study of the film rupture process with inertial effects and arbitrarily large contact angles, in both two and three dimensions. We focus in particular on the evolution of length scales in a perturbed film as it breaks up, and the spatial organization of the resulting drops. We compare our results to recent experiments, where this instability mechanism has been harnessed for the self-assembly of ordered arrays of metallic nanoparticles (ACS App. Mat. and Int., 2014, 6, 5835).

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