Modeling and computation of nanoscale films including thermal effects

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This project is focused on fluid dynamics simulation and modeling involving liquid metal assembly on the nanoscale. The problem will be approached by developing and implementing novel models and computations with complementary experiments targeted to test and validate the models via direct comparison. The experiments are carried out by collaborating group at U. Tennessee led by P. Rack. The numerical findings will be augmented by the results of asymptotic long-wave theory. The proposed work explores complex three dimensional geometries, liquid metal/substrate interactions, and thermal effects where nanoscale thermal gradients will be imposed via temperature dependent material properties.

Significant progress has been recently reached in understanding the dynamics of liquid metals on the nanoscale, leading to exploiting their flow instabilities for self- and direct-assembly. However, the results were obtained mainly by using the long-wave theory whose validity is unclear when the problem under consideration is characterized by large contact angles as well as fast evolution which may lead to appreciable inertial effects. Therefore, to fully understand the dynamics, as well as the limitations of the long-wave approach, it is crucial to develop direct numerical methods for solving the Navier-Stokes equations. The methods that will be developed are based on Volume of Fluid approach, that will also incorporate moving contact lines as well as the potentials describing liquid-solid interaction. The computations will be carried out using adaptive mesh refinement in a parallel computing environment. A distinguishing feature of the proposed project is the immediate and direct comparison of computational and long-wave results with the experimental ones. The theoretical, computational, and experimental work will drive each other, with theoretical predictions directly checked by targeted experiments, and subsequently these experiments will be used to develop more accurate theoretical description of the instabilities and transport of nanoscale liquid metals.

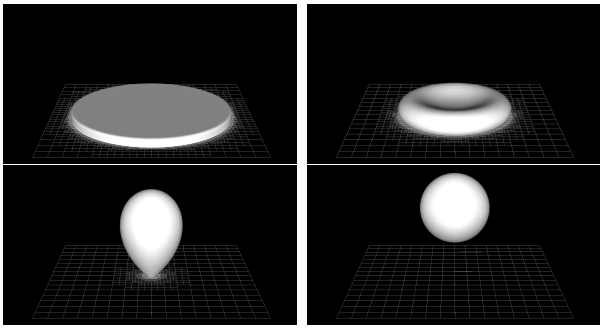

Figure 1: Volume of Fluid based simulations of detaching liquid drops (From Afkahami and Kondic, Phys. Rev. Lett. **111** 034501 (2013)).