PH.D. DISSERTATION DEFENSE ANNOUNCEMENT

METHODS FOR THE DIRECT SIMULATION OF NANOSCALE FILM BREAKUP AND CONTACT ANGLES

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ABSTRACT

This thesis investigates direct simulation of fluids with free surfaces and contact lines, with a focus on capturing nanoscale physics in a continuum based computational framework. Free surfaces and contact lines have long presented some of the most challenging problems in computational fluid dynamics. Extensive progress has been made in recent years, and a wide variety of different methods are currently employed for direct simulation in these contexts. The complexity of the full governing equations for such flows poses significant challenges in terms of analytical techniques, and leads to lengthy computational times for direct simulations. For these reasons, reduced models are preferable in many contexts, even when it is not clear that such reduced models strictly apply.

Recent advances in nanotechnology motivate the comparison between direct simulations and reduced models by presenting situations in which each possesses advantages; these experiments involve the deposition of nanoscale flat metallic structures onto a surface with unprecedented precision, the almost instantaneous liquefaction of which leads to new initial liquid configurations which have been previously impossible to achieve in an experimental setup. The mechanisms that lead to the instability of these structures are a combination of classical liquid instability (such as Rayleigh-Plateau), novel capillary instabilities driven by the initial geometry, and nanoscale physics.

This study begins by examining the differences in qualitative behavior between direct numerical simulation of the full equations and a particular reduced model in the context of wetting and dewetting of drops. Afterwards, a specific initial liquid geometry is presented, the breakup of which requires direct numerical simulation in order to explain the experimental behavior. A parameter study of this geometry demonstrates that it offers a rich variety of dynamics; the breakup of the geometry is found to result in nanoparticle arrangements previously unobtainable using similar techniques, and through careful tuning of the parameters the end state of the breakup can be various combinations of metallic filaments and nanoparticles. While such instabilities are driven by surface tension, an important class of thin film instability is driven by intermolecular fluid/solid interactions. A numerical method is developed which, for the first time, permits the explicit inclusion of this fluid/solid interaction in the context of direct numerical simulations. This method not only allows for modeling and simulating film breakup, but additionally yields a numerical method for the simulation of contact angles as well.