Nanohydrodynamic simulations: An atomistic view of the Rayleigh Taylor instability.

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Commentary by Leo Kadanoff, University of Chicago.

This article reflects a major achievement of the Stockpile Stewardship Program of the Weapons Laboratories of the U.S. Department of Energy. The program, among other things, develops methods of large scale computing and tests their reliability and their effectiveness in helping understand important scientific and engineering problems. In this paper, the method is the use of molecular dynamics techniques for the study of hydrodynamic systems at the nano-scale. (See also the earlier molecular dynamics study of nanoscopic jets by Moseler and Landman, reference 34 in this paper.) Here, the method is being tested for its application to the hydrodynamic instability which arises when a heavy fluid is accelerated into a lighter one. This Rayleigh-Taylor (R-T) instability has been a major focus of the stewardship program, with no fewer than ten different published studies being devoted to this topic. (See the discussions in references 13, 14 and 31 of this paper.) This is one of several vexing fluid instabilities which might be important in macroscopic situations in, for example, fusion reactors. The present paper apparently has two goals, a. to develop and test a method which might be applicable to nano-scale studies and b. to shed light on studies of this instability at the macro scale.

The first goal is reached in an admirable fashion. The paper includes studies with up to a billion particles, and also systems with fewer, and shows how the nano-scale phenomena can reflect averaged motion qualitatively similar to that in macroscopic fluids.

Although many earlier studies, including the classic work of Alder and Wainwright, have shown fluid behavior in small systems, this particular nano-system might have special problem because of its sharp interfaces, tremendously enhanced gravity, and especially its hydrodynamic instabilities. These aspects of the system might cause its behavior to be substantially modified by the strong fluctuations characteristic of small systems. Ref. 34 shows that, in the case of jet behavior, fluctuations dominate the late-time interface shape.

Similarly, in this Rayleigh-Taylor situation, the unstable part of the linear stability behavior is dominated by fluctuations. This domination makes any comparison with the earlier macroscopic R-T studies rather problematical. The earlier studies themselves are, taken together, quite problematical. They split into two groups roughly equal in technical sophistication, but differing by a factor of two in their answers for the fluids' penetrating power. The present paper seems to claim that it shows a quantitative validation of its methods against these earlier studies involving macroscopic hydrodynamics, but this claim is made at the expense of rejecting the results of half of the previous studies. However, most of the previous stewardship R-T studies are suspect because they are quite close to the zero-surface-tension, zero-viscosity limit in which the problem is mathematically ill-defined. Close to this limit, any study is very delicately dependent upon calculational and observational methodology.

Consequently, I cannot accept the validation claim of the present paper, but I am happy to accept the idea that the method provides quantitative information about the nano-domain and qualitative information about the developed instabilities in the macroscopic. Unfortunately, the stewardship program studies seems to have shown that present-day computations cannot yet give reliable quantitative answers for problems involving well-developed macroscopic interface instabilities.