Discretization and Modeling of Deformable Boundary Problems

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Summary

Dynamic deformable boundaries are a major challenge in numerical methods for simulating the response of complex soft materials and their interaction with fluids. These are key features in many DOE applications including low-dose radiation damaged cells and elastic structures interacting with gases and viscous flows. This project develops new numerical methods with improved accuracy near time-dependent boundaries. The techniques have been demonstrated by simulations of fluid dynamic instabilities which revealed previously unknown physical scaling regimes.

Existing numerical methods for flow in deformable domains have difficulties resolving flow features near moving boundaries. Researchers at LLNL are designing new mathematical models and numerical methods for flow dynamics involving deformable boundaries with applications to shape-changing materials and biological cells interacting with a fluid through their deformable membranes.

Another important application is gravity driven soap film flow experiments where a very thin liquid layer of micron thickness, a few inches in width and a few feet in length is used as a “table top wind tunnel.” Theoretical models of this flow were developed but direct simulation of the full three-dimensional liquid layer with free boundaries is currently intractable. The lack of simplified mathematical models of this flow has limited the usefulness of this powerful experimental technique. To address this problem, LLNL mathematicians utilized a systematic perturbation analysis to reduce the problem to a new two-dimensional model that is equivalent in form to the compressible Navier-Stokes equations which in turn are immensely important in DOE applications. This work establishes a practical new computational model with a firm theoretical foundation. The model allows the validation of large scale flow solvers through soap film flow experiments which are relatively simple to characterize completely.

Fig. 1 shows a simulation of planar compressible flow using the new soap film model. The thickness of the film is shown in a downward flow past a row of cylinders.

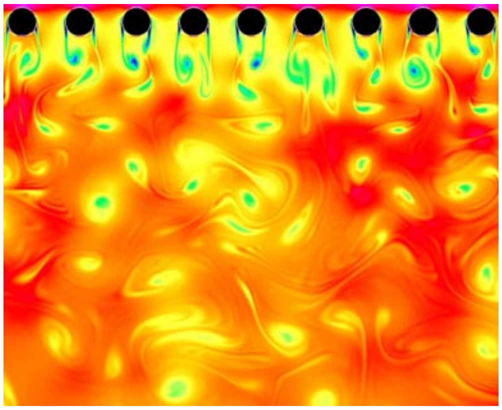

Figure 1. Film thickness in a simulation of a soap film model that allows validation of viscous effects in compressible flow solvers.

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Improvements in algorithms for studying fluid dynamic instabilities are of central importance to the DOE mission. An excellent test case for this is the Saffman-Taylor "viscous fingering" instability. Viscous fingering is a prototypical free-boundary problem that shares many of the difficulties often encountered in simulations of dynamic boundaries in fluids. Advanced algorithms development at LLNL enabled new reference simulations of unprecedented scale for the Saffman-Taylor instability. These simulations illustrate the effect Moore's law has on simulations of fluid dynamic interfacial instabilities: While computing power has increased 100x in the past ten years, far more important has been the discovery of algorithms with optimal runtime complexity under Office of Science funding. The simulations shown in Fig. 1 reached a new asymptotic scaling regime that can be matched to an experimentally measured power-law characterization of the evolving interfacial shape.

Work is in progress to develop a new numerical approach for problems involving three-dimensional bulk deformable objects. The key idea is to couple a structured computational grid that yields excellent accuracy and efficiency with thin boundary adapted unstructured volume grids that maximize robustness and geometric flexibility. This new "prismatic / Cartesian grid method" has potential for broad impact on modeling the response of soft materials in high speed flows. This work is motivated by a need to enhance our understanding of the fundamental properties of biological cells damaged by low-dose radiation, and to improve simulations of the response of elastic structures interacting with gases and other solids.

This project is also committed to educating the next generation of computational scientists. A new intensive course was designed at LLNL to teach the fundamentals of the numerical methods that are at the core of many DOE applications. This course was lectured to visiting faculty and to graduate student research fellows participating in the LLNL 2006 summer program.

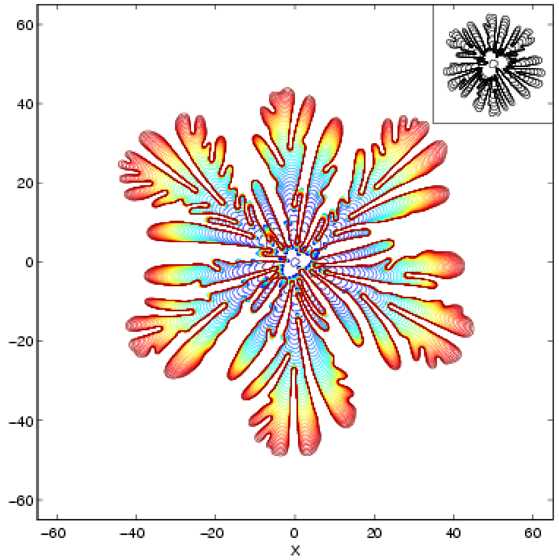

Figure 1 The world's largest simulation of "viscous fingering" to date demonstrates how optimal computational algorithms enable new scientific discoveries. This simulation is a significant improvement over previous state-of-the-art (inset).

References:

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