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SPECTRAL BOUNDARY ELEMENT ALGORITHMS FOR MULTI-LENGTH INTERFACIAL DYNAMICS IN POROUS MEDIA AND MICROFLUIDIC CHANNELS

P. Dimitrakopoulos[1] and N. Boruah[2]

[1] Department of Chemical and Biomolecular Engineering, Bioengineering Program, University of Maryland, USA, dimitrak@umd.edu

[2] Department of Chemical and Biomolecular Engineering, University of Maryland, USA

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The dynamics of droplets and bubbles in confined solid geometries under Stokes flow conditions is a problem of great technological and fundamental interest since it is encountered in a broad range of industrial processes. In the petroleum industry, enhanced oil recovery techniques are strongly dependent on the interaction of oil and water in immiscible two phase mixtures, and the success of such operations depends on the motion and deformation of small oil droplets confined between the walls of porous media. In microfluidic devices, drop motion and sliding on solid channels is commonly used to produce controlled size droplets and for droplet mixing.

Since the pioneering work of Youngren and Acrivos thirty years ago, interfacial dynamics in Stokes flow via the solution of boundary integral equations has developed considerably. The main benefits of this approach are the reduction of the problem dimensionality by one and the great parallel scalability. A lot of research has been done to determine and understand the deformation of droplets and bubbles in viscous flows, both in infinite media as well as in constrained geometries. Considerable progress has also been made in the study of membrane-like interfaces such as those in artificial capsules and erythrocytes.

In this talk, we will present our efforts to develop a series of efficient and highly-accurate interfacial algorithms based on our Spectral Boundary Element implementation for Stokes flow. Our first effort was to develop interfacial spectral boundary element algorithms for the dynamics of three-dimensional droplets and bubbles in Stokes flow based on explicit time integration [1]. The main attraction of this approach is that it exploits all the benefits of the spectral methods (i.e. high accuracy and numerical stability), without being affected by the disadvantage of the spectral methods used in partial differential equations to create denser systems. Our method also exploits all the benefits of the boundary integral techniques, i.e. reduction of the problem dimensionality and great parallel scalability, while its element nature facilitates considerably the incorporation of complicated solid geometries [3].

Despite its unique properties, our novel interfacial algorithm described above still requires that the time step should be sufficiently small (with respect to the space discretization) to ensure numerical stability due to the explicit time integration. This is also a disadvantage of all the current interfacial algorithms in Stokes flow. To avoid this difficulty, we have developed an efficient, fully-implicit time integration algorithm based on a mathematically rigorous combination of implicit formulas with our Jacobian-free three-dimensional Newton method [2]. The resulting algorithm preserves the stability of the employed implicit formula and thus it has strong stability properties which permit the utilization of very large time steps independent of the employed space discretization.

In addition, in our talk we will present our efforts to study efficiently a family of particularly challenging interfacial problems; namely, the case of multi-length interfacial dynamics in Stokes flow. In many interfacial processes, multiple length scales appear and affect the interfacial dynamics. Common examples constitute the drop coalescence process (which, beyond the drop size, also includes the small gap between the interfaces), droplets/cells in close proximity to solid surfaces (as in microfluidic channels, porous media, and the microcirculation) as well as the appearance of tips and necks during large interfacial deformation in strong flows.

Currently the study of multi-length interfacial dynamics in three dimensions constitutes a computational challenge owing to the requirement of extreme numerical accuracy for the accurate determination of the dynamics between the regular (drop-size) scale and the small length scale present in these problems. To overcome this difficulty, we have utilized our Jacobian-free, fully-implicit interfacial spectral boundary element algorithm [2]. This methodology exhibits high accuracy (even with regular grids) due to its spectral nature while its fully-implicit nature makes the employed time step independent of the space discretization and the presence of small length scales. As applications for multi-length interfacial systems, we will present our results for the deformation and motion of droplets in confined solid geometries such as microfluidic channels and porous media.

REFERENCES

[1] Y. Wang and P. Dimitrakopoulos, A three-dimensional spectral boundary element algorithm for interfacial dynamics in Stokes flow. *Phys. Fluids* **18**, 082106 (2006).

[2] P. Dimitrakopoulos, Interfacial dynamics in Stokes flow via a three-dimensional fully-implicit interfacial spectral boundary element algorithm. *J. Comput. Phys.*, **225**, 408–426 (2007).

[3] P. Dimitrakopoulos, Deformation of a droplet adhering to a solid surface in shear flow: onset of interfacial sliding. *J. Fluid Mech.*, **580**, 451–466 (2007).