NON-LINEAR FLUID FLOW/SURFACTANT/INTERFACE DYNAMICS

Antony N. Beris
Department of Chemical Engineering
University of Delaware
Newark, DE 19716
phone: (302) 831-8018 fax: (302) 831-1048 e-mail Address: beris@che.udel.edu
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LONG-TERM GOALS

The goal of this research is the development of a theoretical quantitative understanding of the dynamics of high Reynolds number free-surface flows under large free-surface deformations in the presence of one or multiple surfactants. The long-term goal of this research is to understand the effect of the surfactants on (1) turbulence, (2) waves, (3) slick formation and (4) mass transfer through the free surface.

OBJECTIVES

The objectives of the proposed research are several. First, we are aiming to use a newly developed algorithm for direct numerical simulation of free surface flows with surfactants. This scheme is capable of simulating two-dimensional flows with high Reynolds numbers, accommodating nonlinear free surface deformation in the presence of one or multiple interacting surfactants. We want to focus on improving the understanding of the nonlinear flow/free-surface/surfactant interactions of a surfactant-contaminated free-surface with a vortex, with or without the presence of waves. Second, we want to use the simulation results to evaluate a variety of models for the surfactant behavior. In particular, through comparison with experimental data, we want to investigate the extent of microscopic detail needed to be present in the surfactant model in order to enable an at least qualitative description of the dynamic surfactant behavior.

APPROACH

The approach followed for the accurate and computationally efficient evaluation of the flow, free-surface deformation and surfactant concentration involves to development of a direct numerical simulation capability based on a fully spectral spatial discretization and a conformal mapping of the flow domain into a regular parallelepiped. The conformal mapping is key in order to preserve the computational efficiency of the proposed numerical technique since it allows the use of computationally efficient fast Poisson algorithms for the solution of the Poisson and Helmholtz problems generated from the time-integration of the flow and surfactant concentration evolution equations. The numerical time-integration approach for nonlinear free-surface flows in the presence of insoluble surfactants is a recently developed, fully implicit scheme based on an iterative predictor-corrector method. This approach has also led to very efficient numerical schemes for stationary boundary problems, where it has been extended to three dimensions. In addition, the capability of simulating soluble surfactants can now be incorporated in a straightforward manner. We have also gained extensive experience in parallel computing and have the capability of performing our simulations in powerful parallel computing environments through very efficient implementations of our algorithms, which are linearly scalable with the number of processors. Thus, we are in a unique position to perform efficient simulations of free-surface flows with surfactants, accommodating fully nonlinear free-surface deformations, with very high accuracy.

WORK COMPLETED

During the past year, we completed the development of an algorithm for simulation of fully non-linear free-surface flows in the presence of surfactants. This algorithm exhibits almost linear scalability in computational cost ($N\log_2 N$) with the number of unknowns, N. It is based on a fully implicit iterative predictor-corrector time-integration scheme, pseudoconformal mapping of the flow-domain to the computational domain and a spectrally preconditioned iterative conjugate gradient

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14. ABSTRACT
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solver. Implicit time-integration was necessary for stability given the highly nonlinear boundary conditions.

The concept behind the algorithm is simple and its implementation is as follows. An Adams-Bashforth scheme is used for the non-linear terms in the predictor step and an Adams-Moulton scheme for the corrector step. One recalculates the non-linear terms at the current time-step by repeating the corrector step in an iterative fashion till convergence with high tolerance (e.g. 10^{-12}). This algorithm is only 2-3 times more expensive than the mixed scheme and has the advantage that the initial guess need not satisfy the continuity equation very well, allowing for more freedom than a conventional Newton-Raphson approach. Of course, the main disadvantage compared to a full Adams-Moulton scheme using an external Newton-Raphson iteration is that it is not as stable. However, it is adequately stable for use even in free-surface problems. In fact, the corrector step converges faster than the predictor step, since the iterative algorithm starts with a better initial guess. Therefore, the algorithm is actually only a factor of 2 slower than that using a mixed time-integration scheme.

The kinematic condition is implemented along with the orthogonality constraint in the algorithm that computes the time-derivatives of the mapping. This is achieved by solving iteratively two separable Poisson equations, using a similar method to that in Dimitropoulos *et al.* (1998), with the following (coupled) boundary conditions:

$$\frac{\partial y}{\partial t}=\left(u_\eta-\frac{\partial x}{\partial t}\frac{\partial x}{\partial \eta}\right)\Big/\frac{\partial y}{\partial \eta},$$

$$\frac{\partial}{\partial \eta}\left(\frac{\partial x}{\partial t}\right)=\left(-\frac{\partial}{\partial \xi}\left(\frac{\partial x}{\partial t}\right)\frac{\partial x}{\partial \eta}-\frac{\partial}{\partial \xi}\left(\frac{\partial y}{\partial t}\right)\frac{\partial y}{\partial \eta}-\frac{\partial}{\partial \eta}\left(\frac{\partial y}{\partial t}\right)\frac{\partial y}{\partial \xi}\right)\Big/\frac{\partial x}{\partial \xi}.$$

Once the time-derivatives of the mapping are known, we can then find the actual mesh by integrating in time. To enforce orthogonality over the time-integration error, we fit the top boundary calculated through the time-integration to a Fourier series and then use this Fourier series as a functional representation in the mapping algorithm for a given surface (described in Dimitropoulos *et al.*, 1998). We then proceed to solve for the flow problem with a known mesh at the new time-step. This is made robust through a predictor-corrector scheme. Initially, we use explicit integration for the mesh. We solve for the velocities and then recalculate the time-derivatives of the mesh with this new velocity and use implicit integration for the mesh. We proceed to solve again for the velocity field. Once this first corrector step is completed, we repeat it until the values we obtain do not change. This is necessary since we have decoupled the solution of the mesh from the solution of the flow problem. This would not be possible using the fully implicit scheme with an external Newton-Raphson iteration. This approach allows us to solve the surface diffusion equation for the surfactant species and to implement the full nonlinear free-surface boundary conditions without needing to change substantially the preconditioned conjugate gradient solver.

The surface diffusion equation can be solved during each iteration in a straightforward manner, right after the coordinates are updated through the mapping algorithm. The equation governing the transport of an insoluble surfactant on an interface takes the following form when expressed in the orthogonal curvilinear coordinate system that is utilized in this work, where Γ is the concentration of the surfactant on the interface and Pe_s the surface Peclet number.

$$\frac{\partial \Gamma}{\partial t}+\frac{\partial \Gamma}{\partial \xi}\frac{\partial \xi}{\partial t}+\frac{1}{h_\xi^2}\left(u_\xi\frac{\partial \Gamma}{\partial \xi}+\Gamma\frac{\partial u_\xi}{\partial \xi}-\frac{\partial \ln h}{\partial \xi}\Gamma u_\xi\right)=\frac{1}{Pe_s h_\xi^2}\left(\frac{\partial^2 \Gamma}{\partial \xi^2}+-\frac{\partial \ln h}{\partial \xi}\frac{\partial \Gamma}{\partial \xi}\right)$$

The above equation is solved assuming the velocity field is known, just as is performed for the mapping. In fact, given the structure of the algorithm this is the most natural way to treat the convection-diffusion problem on the interface; the surface concentration is a property of the interface, exactly like its shape. Finally, due to the lower dimensionality of this equation compared to the

momentum equations in the bulk, it is possible to use a simple direct solver and a fully implicit Adams-Moulton time-integration scheme to solve the system of algebraic equation that results after pseudospectral discretization using Fourier collocation. The cost of solving this equation does not affect the overall computational cost of the algorithm.

Once the surface concentration is known, one can calculate the surface tension through a constitutive relationship. We have chosen to use a nonlinear, Langmuir type relationship which is adequate to capture local surfactant saturation effects. The equation considered is

$$\sigma = 1 + Ma(1+\beta)\ln\left(\frac{1+\beta-\Gamma}{\beta}\right)$$

where Ma is the Marangoni number, which represents the ratio of the interfacial tension gradient forces to bulk viscosity forces and the β is a parameter that represents nonlinear packing effects. When β is very large, ideal behavior (linear variation of surface forces with concentration) is recovered.

For the free-surface boundary conditions, we utilize the Boussinesq-Scriven model for the surface stress, which assumes linear dependence of the stress on the strain rate. When we express the boundary conditions in the pseudoconformal coordinate system utilized in this work they take the form:

$$-p\,\mathrm{Re}+\frac{2M}{h_\xi^2}\left(\frac{\partial u_\eta}{\partial\eta}-\frac{\partial \ln h}{\partial\eta}u_\eta+\frac{1}{M}\frac{\partial \ln h}{\partial\xi}u_\xi\right)=\frac{2H\sigma}{Ca}+\frac{2MH}{h_\xi^2}\left(\frac{\partial u_\eta}{\partial\eta}-\frac{\partial \ln h}{\partial\eta}u_\eta+\frac{1}{M}\frac{\partial \ln h}{\partial\xi}u_\xi\right)\quad\text{normal stress}$$

$$\frac{\sqrt{M}}{h_\xi^2}\left(\frac{\partial u_\eta}{\partial\xi}+\frac{\partial u_\xi}{\partial\eta}-2\frac{\partial \ln h}{\partial\xi}u_\eta-2\frac{\partial \ln h}{\partial\eta}u_\xi\right)-\frac{1}{h_\xi Ca}\frac{\partial\sigma}{\partial\xi}+\frac{Bo}{h_\xi^2}\left[-3\frac{\partial \ln h}{\partial\xi}\frac{\partial u_\xi}{\partial\xi}+M\frac{\partial \ln h}{\partial\eta}\frac{\partial u_\eta}{\partial\xi}+2\left(\frac{\partial \ln h}{\partial\xi}\right)^2u_\xi\right.$$

$$\left.-\left(\frac{\partial^2 \ln h}{\partial\xi^2}\right)u_\xi+M\frac{\partial^2 \ln h}{\partial\xi\partial\eta}u_\eta-2M\frac{\partial \ln h}{\partial\xi}\frac{\partial \ln h}{\partial\eta}u_\eta+\frac{\partial^2 u_\xi}{\partial\xi^2}\right]=0\quad\text{tangential stress,}$$

where Ca is the capillary number, Bo is the Boussinesq number and H is the mean curvature of the interface. We implement these boundary conditions in the preconditioner, along with the divergence-free condition after transforming them into the following set of equations:

$$-p^i=\frac{2M}{K\,\mathrm{Re}}\left[\left(\frac{\partial u_\eta}{\partial\eta}\right)^i+\left(-\frac{\partial \ln h}{\partial\eta}u_\eta+\frac{1}{M}\frac{\partial \ln h}{\partial\xi}u_\xi-p\left(\frac{h_\xi^2}{1+HBo}-K\right)\frac{\mathrm{Re}}{2M}\right)^{i-1}-RBC1\right]$$

$$\left(\frac{\partial u_\xi}{\partial\eta}\right)^i=\left(-\frac{\partial u_\eta}{\partial\xi}+2\frac{\partial \ln h}{\partial\xi}u_\eta+2\frac{\partial \ln h}{\partial\eta}u_\xi\right)^{i-1}+\frac{Bo}{h_\xi^2}\left[-3\frac{\partial \ln h}{\partial\xi}\frac{\partial u_\xi}{\partial\xi}+M\frac{\partial \ln h}{\partial\eta}\frac{\partial u_\eta}{\partial\xi}+2\left(\frac{\partial \ln h}{\partial\xi}\right)^2u_\xi\right.$$

$$\left.-\left(\frac{\partial^2 \ln h}{\partial\xi^2}\right)u_\xi+M\frac{\partial^2 \ln h}{\partial\xi\partial\eta}u_\eta-2M\frac{\partial \ln h}{\partial\xi}\frac{\partial \ln h}{\partial\eta}u_\eta+\frac{\partial^2 u_\xi}{\partial\xi^2}\right]^{i-1}+RBC2$$

$$\left(\frac{\partial u_\eta}{\partial\eta}\right)^i=-\frac{1}{M}\left(\frac{\partial u_\xi}{\partial\xi}\right)^{i-1}+RBC3.$$

The constant K is the average of $h_\xi^2/(1+HBo)$, RBC1, RBC2, RBC3 are the residuals of the boundary conditions calculated in the conjugate gradient level and i is the index of the Concus and Golub type iteration performed in the preconditioner. This scheme is constructed so that the influence matrix method can be efficiently implemented in order to enforce the divergence-free condition.

RESULTS

We have validated the algorithm by comparing its predictions against those of linear theory of wave damping in the presence of surfactants. This work will be communicated in a series of forthcoming articles (see Dimitropoulos 1999c) which will include the methodology and results in a comprehensive fashion. Here, we present briefly results from simulations of a purely elastic interface without viscous or molecular diffusion effects. In the case that surfactants are present, two modes of motion exist, transverse as well as longitudinal waves. Tables 1 and 2 present a comparison of linear theory with simulation results for damping of transverse and longitudinal waves. The initial amplitude was equal to 10^{-3} in a channel 2 units deep and 1 unit wide, $Re=10^{4}$ (based on the half-depth and the gravity), $Ca=10^{-1}$ (corresponding to water), Ma=4/9, Bo=0, $Pe_s=10^{18}$ and the time-step was equal to 10^{-3}.

	Linear Theory	Numerical Simulation
Damping Factor	-0.062571	-0.062599
Period of Oscillation	2.43798	2.43815

Table 1: Damping of transverse waves: Comparison of simulations with linear theory.

	Linear Theory	Numerical Simulation
Damping Factor	-1.222236	-1.298954
Period of Oscillation	2.98021	2.88204

Table 2: Damping of longitudinal waves: Comparison of simulations with linear theory.

It can be readily observed that the simulations agree well with theory. It should be noted that the larger discrepancy in the results for longitudinal waves is due to the sensitivity of the simulations in the initial guess that makes the initial motion, which is mostly of longitudinal character, to evolve and include a small superimposed contribution of the transverse mode. We must emphasize here that we found that the flow field that corresponds to each mode is quite different. The horizontal velocity for longitudinal waves in the vicinity of the surface is one order of magnitude greater than for transverse waves. As a result, the pressure distribution also has distinct differences, which persist further away from the surface than the velocity differences. Detailed results that clearly demonstrate the different physics for each type of motion are included in a recent doctoral dissertation supported by this project and will be presented in a series of future publications.

IMPACT/APPLICATIONS

We have developed a computationally efficient numerical scheme for solving spectrally, two-dimensional, time-dependent free-surface flows in the presence of insoluble surfactants. The implementation was such that the almost linear scalability and exponential convergence with mesh refinement characteristics are retained. An orthogonal mapping algorithm, an efficient and robust iterative solver incorporating the influence matrix method for satisfying the incompressibility condition and an iterative predictor-corrector implementation have been developed. The algorithm is parallelizable in a straightforward fashion and exhibits linear scalability of its performance with the number of processors used. This is the first time in our knowledge that a fully spectral method for simulation of fully nonlinear free-surface flows with surfactants has been developed. This method has unique capabilities to elucidate the complex phenomena that occur in situations where there is nonlinear coupling of fluid flow, interface deformation and mass transport of surfactants.

TRANSITIONS

The main development of this work along with that performed over the past 5 years is a quite general in applicability set of algorithms, which extend the use of fully spectral methods to flows within moderately complex geometries. The tools developed in this work i.e. the pseudoconformal mapping and the efficient spectral preconditioner are also applicable to other computational fluid mechanics and transport phenomena problems. All of these are expected to find significant use within the computational fluid dynamics community, since their possible applications span a quite wide area.

RELATED PROJECTS

The core of the spectral numerical method, after suitable modification, has been successfully used in direct numerical simulations (DNS) of turbulent viscoelastic flows in a joint University of Delaware - NRL effort for the investigation of

polymer-induced turbulent drag reduction. There has been substantial progress after our latest simulations in the CRAY-Origin2000 at National Center for Supercomputing Applications (NCSA). This work has produced so far four publications (Sureshkumar *et al.*, 1997; Dimitropoulos *et al.*, 1998b, Beris and Dimitropoulos, 1999a, Dimitropoulos *et al.*, 1999b) and is being continued to study further the phenomenon of drag reduction. The implementation in multiprocessor environments of the codes developed in the current project has been greatly facilitated from the above-mentioned experience.

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