INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS, VOL. 13, 691–698 (1991)

VARIATIONAL FORMULATION OF THREE-DIMENSIONAL VISCOUS FREE-SURFACE FLOWS: NATURAL IMPOSITION OF SURFACE TENSION BOUNDARY CONDITIONS

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SUMMARY

We present a new surface-intrinsic linear form for the treatment of normal and tangential surface tension boundary conditions in C^0-geometry variational discretizations of viscous incompressible free-surface flows in three space dimensions. The new approach is illustrated by a finite (spectral) element unsteady Navier–Stokes analysis of the stability of a falling liquid film.

KEY WORDS Curvature Finite element method Free surface flow Navier–Stokes equations Spectral element method Surface tension Three-dimensional Variational form Viscous incompressible flow

1. INTRODUCTION

Multifluid and free-surface flows with surface tension play an important role in a wide variety of engineering and natural systems. Examples of ubiquitous multifluid phenomena include the flow of bubbles and droplets,[1] the evolution of free and interfacial surface waves[2] and multiphase heat transfer.[3] The numerical solution of these difficult non-linear free-boundary problems is increasingly being addressed by front-tracking finite element methods;[4–8] finite element discretizations are attractive not only due to their geometric flexibility but also due to their variational origin. In particular, the variational treatment of divergence-of-flux physical laws reduces the continuity requirements on the solution space and naturally generates complex flux boundary conditions. In this paper we exploit this variational advantage in the treatment of surface tension boundary conditions in *three* space dimensions.

Most work to date on three-dimensional surface tension problems considers effectively inviscid static situations (the Young–Laplace equation), in which a variational form based on the divergence of the surface normal is used to generate the proper pressure jump across the free surface.[9] This variational form has the important advantages of lowering the order of derivatives on geometric factors and of naturally generating contact angle boundary conditions. However, the divergence of the surface normal method also has several disadvantages: the variational form generates the curvature, not the curvature–normal product required in viscous analysis; the variational form does not generate the tangential surface tension boundary condition; the method requires a global rather than a surface-intrinsic co-ordinate system.

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0271-2091/91/160691-08$05.00

Received 12 March 1990
Revised 10 December 1990

We present here a new linear form for surface tension which eliminates the problems associated with the divergence of the surface normal approach. The new method is based on the strong-form surface Laplacian for curvature described in References 10 and 11 and represents an extension to *three* space dimensions and variable surface tension of Ruschak's[12] variational treatment of two-dimensional surface tension problems. We present the new form in Section 2, an example of its application in Section 3 and brief conclusions in Section 4.

2. FORMULATION

We consider viscous unsteady incompressible flow of a Newtonian fluid in a three-dimensional time-dependent domain Ω. The domain boundary $\partial\Omega$ is decomposed as $\partial\Omega=\partial\Omega_0\cup\partial\Omega_\sigma$, with Dirichlet no-slip boundary conditions imposed on $\partial\Omega_0$ and surface tension traction boundary conditions[13,14] imposed on $\partial\Omega_\sigma$. For the current formulation we further require that $\partial\Omega_\sigma$ be either closed (e.g. a bubble, as shown in Figure 1(a)) or periodic (e.g. a wave train, as shown in Figure 1(b)). The governing equations are then

$$\rho(u_{i,t}+u_j u_{i,j})=[-p\delta_{ij}+\mu(u_{i,j}+u_{j,i})]_{,j}+f_i \quad \text{in } \Omega, \tag{1a}$$

$$u_{i,i}=0 \quad \text{in } \Omega, \tag{1b}$$

$$u_i=0 \quad \text{on } \partial\Omega_0, \tag{1c}$$

$$N_i[-p\delta_{ij}+\mu(u_{i,j}+u_{j,i})]N_j=\sigma\kappa \qquad \text{on } \partial\Omega_\sigma, \tag{1d}$$

$$t_i[\mu(u_{i,j}+u_{j,i})]N_j=(t_i\sigma_{,i}) \quad \text{on } \partial\Omega_\sigma, \tag{1e}$$

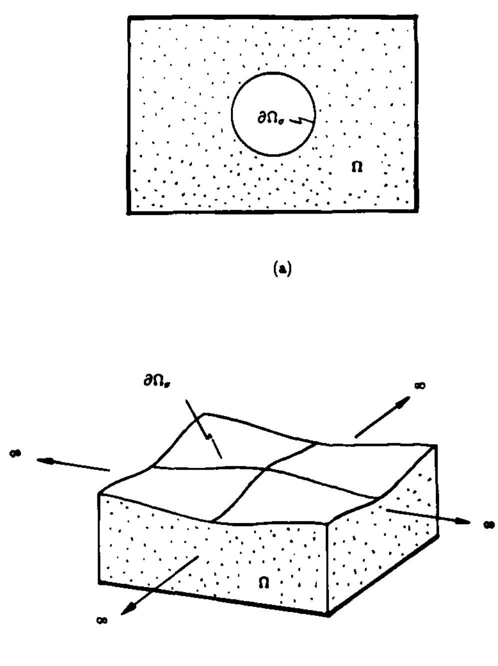

Figure 1. Traction surfaces $\partial\Omega_\sigma$ are considered either (a) closed or (b) periodic

where u_i is the velocity, p is the pressure (relative to zero ambient), f_i is the body force, ρ is the density, μ is the viscosity and δ_{ij} (or δ^i_j) is the Kronecker delta symbol. The following quantities are defined on the free surface $\partial\Omega_\sigma$: σ, the surface tension coefficient, N_i, the outward unit normal; t_i, any tangent vector; and κ, twice the mean curvature.

We shall use notation and conventions: italic indices range from 1 to 3; a subscript indicial comma denotes derivative (e.g. $u_{i,t}=\partial u_i/\partial t$, $u_{i,j}=\partial u_i/\partial x_j$); and repeated italic indices are summed from 1 to 3 (e.g. $u_{i,i}=u_{1,1}+u_{2,2}+u_{3,3}$). In order to avoid subscript proliferation, we shall on occasion use Gibbs notation, with $u_i=\mathbf{u}$ and $u_iv_i=\mathbf{u}\cdot\mathbf{v}$. Since equation (1) is in reference to a Cartesian co-ordinate system, we need not distinguish between covariant and contravariant components of vectors and tensors; this will not be the case for the surface-intrinsic quantities defined below. Note that since σ is defined only on $\partial\Omega_\sigma$ and not in Ω, $\sigma_{,i}$ is undefined; $(t_i\sigma_{,i})$ in equation (1e) must therefore be interpreted as the *surface* gradient of the surface tension on $\partial\Omega_\sigma$.

The variational form of equation (1) is given by:[8,15] Find (u_i, p), $u_i\in H^1_0(\Omega)$ and $p\in L^2(\Omega)$, such that

$$\int_\Omega \{\rho v_i(u_{i,t}+u_ju_{i,j})+v_{i,j}[-p\delta_{ij}+\mu(u_{i,j}+u_{j,i})]-v_if_i\}\,\mathrm{d}V-I_\sigma(v_i)=0 \quad \forall v_i\in H^1_0(\Omega), \tag{2a}$$

$$\int_\Omega qu_{i,i}\,\mathrm{d}V=0 \quad \forall q\in L^2(\Omega), \tag{2b}$$

where v_i and q are test functions, $L^2(\Omega)$ is the space of functions which are square integrable, and $H^1_0(\Omega)$ is the space of functions which are in $L^2(\Omega)$, whose first derivatives are in $L^2(\Omega)$ and which vanish on $\partial\Omega_0$.[16] In the remainder of this paper we shall focus our attention on the definition and interpretation of I_σ, the 'linear' form corresponding to natural imposition of the stress boundary conditions (1d) and (1e).

To begin, we assume that the surface $\partial\Omega_\sigma$ can be represented as the sum of K_σ non-overlapping elemental surfaces $\Gamma^{(k)}$:

$$\partial\Omega_\sigma=\bigcup_{k=1}^{K_\sigma}\overline{\Gamma^{(k)}}, \tag{3}$$

where superscript (k) refers to a surface element, with no summation convention implied. The $\Gamma^{(k)}$ are in turn represented as smooth elemental mappings from $\Lambda^{(k)}$:

$$x_i|_{\Gamma^{(k)}}=X^{(k)}_i(r^\alpha), \qquad r^\alpha\in\Lambda^{(k)}, \tag{4}$$

where the $\Lambda^{(k)}$ are local reference surfaces (e.g. triangles or squares) defined by the surface-intrinsic co-ordinates r^α. All Greek indices will refer to surface co-ordinates with range and summation from 1 to 2. The surface decomposition is shown in Figure 2.

We next recall the following standard definitions from differential geometry:[17]

$$\mathbf{g}^{(k)}_\alpha=\mathbf{X}^{(k)}_{,\alpha}, \tag{5a}$$

$$\mathbf{g}^{(k)}_\alpha\cdot\mathbf{g}^{(k)}_\beta=g^{(k)}_{\alpha\beta}, \tag{5b}$$

$$g^{(k)}_{\alpha\gamma}g^{\gamma\beta(k)}=\delta^\beta_\alpha, \tag{5c}$$

$$\mathbf{g}^{\alpha(k)}=g^{\alpha\beta(k)}\mathbf{g}^{(k)}_\beta, \tag{5d}$$

$$g^{(k)}=\sqrt{[\det(g^{(k)}_{\alpha\beta})]}, \tag{5e}$$

$$\kappa^{(k)}\mathbf{N}^{(k)}=(g^{(k)})^{-1}(g^{(k)}\mathbf{g}^{\alpha(k)})_{,\alpha}. \tag{6}$$

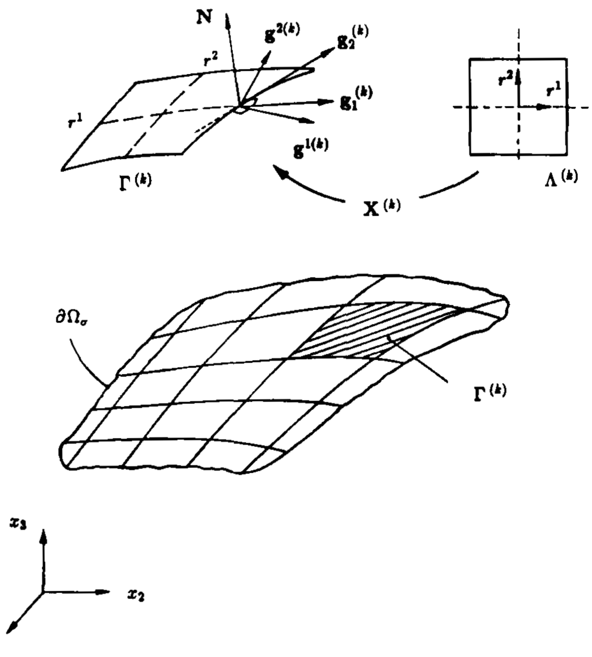

Figure 2. Description of the free surface $\partial\Omega_\sigma$ in terms of elemental surfaces $\Gamma^{(k)}$ represented as mappings $\mathbf{X}^{(k)}$ from reference surfaces $\Lambda^{(k)}$

Here $\mathbf{g}_\alpha^{(k)}$ and $\mathbf{g}^{\alpha(k)}$ are the covariant and contravariant base vectors respectively, $g_{\alpha\beta}^{(k)}$ and $g^{\alpha\beta(k)}$ are the covariant and contravariant metric tensors respectively and $g^{(k)}$ is the Jacobian of the mapping given by equation (4). Equation (6) is the formula of Weatherburn,[10] also found in Reference 11, for the curvature–normal product expressed as a surface Laplacian of $\mathbf{X}^{(k)}$; a related formula is used by Bornside[18] in the finite element treatment of an axisymmetric free-surface flow.

We can now define the 'new' linear form $I_\sigma(v_i)$:

$$I_\sigma(v_i) = -\sum_{k=1}^{K_\sigma} \int_{\Lambda^{(k)}} \sigma \bar{v}^{(k)}_{i,\alpha}\, g_i^{\alpha(k)}\, \mathrm{d}A, \tag{7}$$

where $\bar{v}_i^{(k)} = v_i|_{\Lambda^{(k)}}$ and $\mathrm{d}A = g^{(k)}\mathrm{d}r^1\,\mathrm{d}r^2$. To interpret this form, we perform integration by parts on a surface-elemental basis, arriving at

$$I_\sigma = \sum_{k=1}^{K_\sigma}\left(\int_{\Lambda^{(k)}} \sigma\bar{v}_i^{(k)} (g^{(k)})^{-1}(g^{(k)} g_i^{\alpha(k)})_{,\alpha}\, \mathrm{d}A + \int_{\Lambda^{(k)}} \bar{v}_i^{(k)}\sigma_{,\alpha}\, g_i^{\alpha(k)}\, \mathrm{d}A - \oint_{\gamma^{(k)}} \sigma \bar{v}_i^{(k)} g_i^{\alpha(k)}\, \mathrm{d}n_\alpha\right), \tag{8}$$

where $\gamma^{(k)} = \partial\Gamma^{(k)}$ and $\mathrm{d}n_\alpha = \varepsilon_{\alpha\beta}^{(k)}\,\mathrm{d}r^\beta$, with $\varepsilon_{\alpha\beta}^{(k)}$ the permutation tensor ($\varepsilon_{11}^{(k)} = \varepsilon_{22}^{(k)} = 0$, $\varepsilon_{12}^{(k)} = -\varepsilon_{21}^{(k)} = g^{(k)}$). The last term follows from the surface divergence theorem.[17] If we now assume that the surface $\partial\Omega_\sigma$ is C^1 and recall our restriction that $\partial\Omega_\sigma$ be closed (see Figure 1), the sum of the integrals around the $\gamma^{(k)}$ vanishes. It can then be seen that the two remaining terms in equation (8) are precisely the integrals required for weak imposition of boundary conditions (1d) and (1e) in the variational statement (2a). Thus the single linear form (7) automatically generates both the normal and tangential ('Marangoni') boundary conditions required for viscous analysis.

We assumed a C^1-surface in the preceding analysis only to identify the relevant boundary terms in equation (8). In fact, if we expand our geometry space to include C^0-surfaces, equation (7) is still well defined and the resulting non-zero boundary integrals over $\gamma^{(k)}$ in equation (8) are precisely the weak C^1-conditions (on jumps in $\sigma g_i^{\alpha(k)} g^{(k)}$) required to ensure a meaningful solution. The implies that the form (7) is appropriate in standard C^0-geometry finite element discretizations of equation (2); for example, we can identify the r^α in equation (4) as the local co-ordinate system in the element surface defined by $\Lambda^{(k)}$, and the mapping $X_i^{(k)}$ as an elemental isoparametric transformation. The formulation is entirely surface-intrinsic, with no need to reference global co-ordinates or locally orthogonal systems.

3. NUMERICAL SIMULATION

We present below a brief description of the numerical approach used in the simulation of free-surface flow, followed by a linear stability analysis of an axisymmetric falling viscous film obtained by numerical solution of the time-dependent Navier–Stokes equations (1).

Numerical approach

Our numerical approach[8] is based upon: the variational form (2) and surface tension form (7); spectral element spatial discretization;[19,20] arbitrary Lagrangian–Eulerian description of the time-dependent domain;[8,21] front tracking of the free surface by surface-intrinsic isoparametric co-ordinates; semi-implicit time-stepping procedures;[8] and preconditioned conjugate gradient solution of the fully discrete equations.[19,22]

In the spectral element discretization the computational domain is subdivided into macro-elements and the field variables are approximated by high-order tensor-product polynomial expansions within each macroelement. Variational projection operators and Gauss-type numerical quadratures are used to generate the discrete equations. Convergence is achieved by increasing the order of the polynomial while keeping the number of macroelements fixed. Spectral element methods are optimal in the sense that the approximation error is a multiplicative constant from the best fit in the approximating polynomial subspace.[20]

In the arbitrary Lagrangian–Eulerian (ALE) description the time evolution of the domain geometry is governed by a mesh velocity associated with each material point in the domain.[8] This mesh velocity is independent of the fluid velocity except on the free surface, where the kinematic condition requires that the normal mesh velocity and the normal fluid velocity coincide. Elliptic operators such as the Laplacian or elastostatic equations can be used effectively to extend the mesh velocity into the interior domain such that mesh distortion is minimized. Using the ALE description, consistent treatment of the field variables and their reference configuration can be incorporated, and the time evolution of free-surface position can be accurately tracked.

The issues of temporal discretization and solution algorithm are clearly closely coupled. In the semi-implicit approach[8] those components of the equations (the pressure and viscous elliptic operators) amenable to fast iterative solution such as preconditioned conjugate gradient iteration[23] are treated implicitly, and those components (the convection operator and the coupling of all operators with time-dependent geometry) not readily amenable to fast iterative solution are treated explicitly. The selection of maximally stable high-order semi-implicit time integration schemes is described in detail in Reference 22.

Sample analysis

The axisymmetric film, assumed to be infinitely long in the axial (x_1) direction, is defined by the inner wall radius a, the average film radius b, the average film thickness $h = b - a$, the Reynolds number $R=\rho U_0 h/\mu$ and the Weber number $W=\sigma/\rho h U_0^2$. The scaling velocity U_0 is given by

$$U_0=\frac{\rho g b^2}{4\mu}(\phi^2-2\ln\phi-1), \tag{9}$$

where $\phi=a/b$ and g is the gravitational acceleration. The density ρ, viscosity μ and surface tension σ are all taken to be constant. The geometry and film parameters are shown in Figure 3.

One solution to the governing equations (1) for all R and W is given by a *flat* free surface with

$$\bar{U}_1=\frac{\phi^2-(x_2/b)^2-2\ln(a/x_2)}{\phi^2-2\ln\phi-1}U_0, \tag{10a}$$

$$\bar{U}_2=0, \tag{10b}$$

$$\bar{P}=0, \tag{10c}$$

where x_2 is the radial co-ordinate. In a temporal linear stability analysis we perturb the free surface and equilibrium solution (10) by a sinusoidal disturbance of axial wavelength λ and amplitude η, $\eta \ll h$, and determine whether such a disturbance grows or decays in time. The growth rate of the least stable disturbance for all wavelengths $n\lambda$ (n a positive integer) is denoted γ_r—all quantities will behave as $e^{\gamma_r t}$ for sufficiently long times.

For our sample stability analysis we take the film parameters as $a=1$, $b=2$, $U_0=1$, $\lambda=5\pi$, $W=1$ and $R=1$. We include one wavelength of the film in the computational domain and impose periodic boundary conditions in the axial direction. In order to demonstrate the three-dimensional capability of the formulation, we employ 30 sixth-order *three-dimensional* spectral elements to represent the film; furthermore, a 45° twist is applied to the mesh to ensure that the surface-elemental co-ordinates are non-orthogonal. The resulting spectral element decomposition is shown in Figure 4.

We solve the fully non-linear Navier–Stokes equations from initial conditions comprising the equilibrium flow (10) and a small (2%) free-surface perturbation. The growth rate γ_r is then evaluated from the time history of the L^2-norm of the perturbation velocities as shown in Figure 5. The three-dimensional spectral element calculation predicts a growth rate $\gamma_r=0{\cdot}0484$;

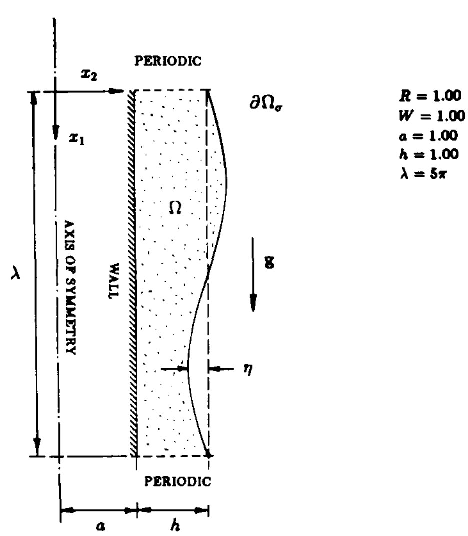

Figure 3. Geometry and flow parameters for linear stability analysis of an axisymmetric falling film

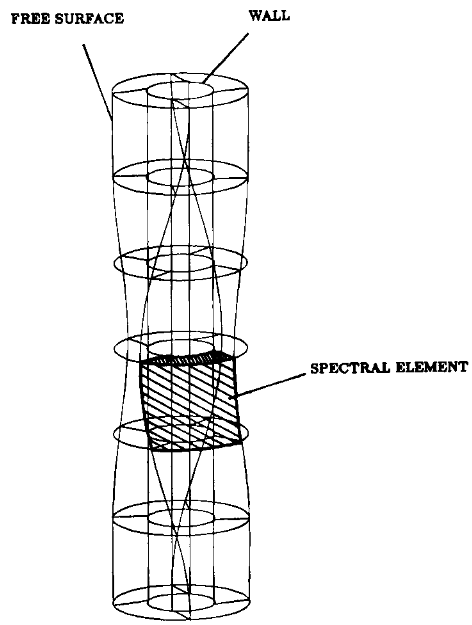

Figure 4. Three-dimensional Legendre spectral element mesh for linear stability analysis of an axisymmetric falling film

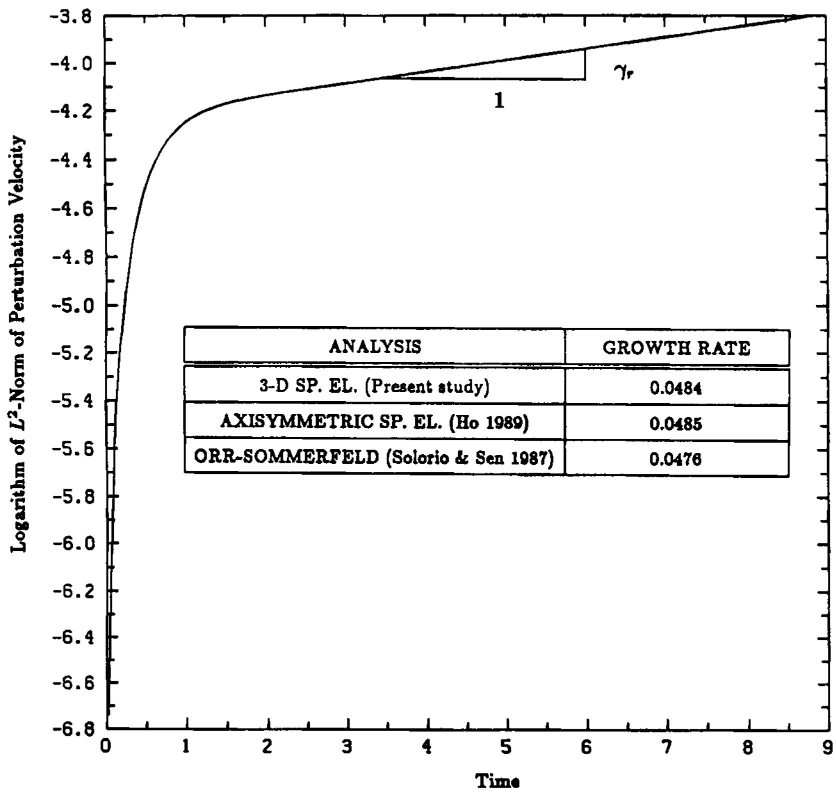

Figure 5. Legendre spectral element prediction of the growth rate of an unstable perturbation to an axisymmetric falling film

this result is in good agreement with the Orr–Sommerfeld solution $\gamma_r = 0{\cdot}0476$ given by Solorio and Sen,[24] as well as the axisymmetric spectral element solution $\gamma_r = 0{\cdot}0485$ given by Ho.[22]

4. CONCLUSIONS

A new variational linear form is presented for the treatment of general surface tension boundary conditions in three-dimensional incompressible viscous free-surface flows. This new form has the following important advantages: first, it provides a consistent treatment for variable surface tension; secondly, it automatically generates (in a weak sense) natural conditions for C^1-continuity of the free-surface geometry; and lastly, it is entirely surface-intrinsic and thus well suited for discretization using finite element techniques. Future work will include extension of the formulation to open domains involving contact angle boundary conditions.

ACKNOWLEDGEMENTS

We would like to thank Professor Robert A. Brown of MIT for his contributions to this work. We would also like to acknowledge helpful discussions with Professor Stephen H. Davis of Northwestern University and Dr. David E. Bornside of MIT. This work was supported by ONR and DARPA under Contract N00014-89-J-1610.

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