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A Finite Element Method for Capillary Surfaces with Volume Constraints

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Capillary surfaces with prescribed volume are determined numerically. The obstacles that confine the given amount of liquid may be planes in space arbitrarily chosen. Parameters of the problem are the Bond number, the contact angle, and the volume. Results for several examples are presented, such as a drop in a corner and on an edge.

1. INTRODUCTION

In this paper we describe a numerical method to determine approximately the shape of the domain Ω filled by a liquid of given volume V_0 which is confined to a given container Φ the walls $\partial\Phi$ of which are planes. It is assumed that the liquid is at rest under the influence of surface tension, adhesion forces to the walls, and gravity. In general, this problem does not have unique solutions; there may be infinitely many. Therefore, we restrict the problem in that we impose certain assumptions on the geometric configuration in space. A model for the problem goes back to Laplace [7], who stated that on a capillary surface the difference of the pressures on either side is twice the product of the surface tension and the mean curvature. The modern mathematical theory of capillary surfaces is dealt with in [1, 2]. This is closely related to the theory of minimal surfaces, cf. [9].

Numerical techniques for the calculation of capillary surfaces were developed by many authors in the case where the surface is a graph of a function, cf. [8]. A systematic study of problems which reduce to ordinary differential equations was recently carried out in [5].

Here we introduce a finite element method (see Section 3) which also works in the cases of parameterized surfaces. The basic idea is similar to what was used in [4, 12] for the Plateau problem.

2. THE VARIATIONAL PROBLEM AND ITS EULER–LAGRANGE EQUATION

First of all, we introduce the notations necessary to describe the problem (Fig. 2.1).

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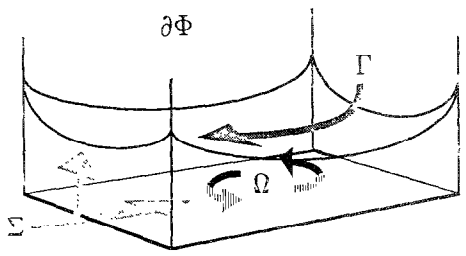

Figure 1

Notations.

Φ = container = (not necessarily bounded) domain in space $\mathfrak{R}^3$

$\partial\Phi$ = walls of the container = union of a finite number of planes

Ω = domain occupied by the liquid, $\Omega \subset \Phi$

$\partial\Omega = \text{clos}(\Gamma) \cup \text{clos}(\sum)$ = boundary of Ω

Γ = capillary surface = free surface of Ω, $\Gamma \subset \text{int } \Phi$

$\sum$ = wetted surface on the walls of the container, $\sum \subset \partial\Phi$

V = volume of Ω

V_0 = prescribed volume

S = area of Γ

F = area of $\sum$

G = gravitational energy

E = total energy

$b = g\rho l^2/\sigma$ = Bond number

g = gravitational acceleration

ρ = density of the liquid

l = characteristic length of Φ

σ = surface tension

β = relative adhesion coefficient

$x = (x_1, x_2, x_3)$ = point in space $\mathfrak{R}^3$

The total energy in dimensionless form is given by

$$E = S + bG + \beta F, \tag{2.1}$$

where

$$S = \int_{\Gamma} d\Gamma, \qquad G = \int_{\Omega} x_3 \, d\Omega, \qquad F = \int_{\Sigma} d\Sigma, \tag{2.2}$$

cf. [2].

The variational problem characterizing equilibria is

$$E^* = \min\{E : \Omega \subset \Phi,\ V = V_0\} \tag{2.3}$$

with

$$V = \int_{\Omega} d\Omega. \tag{2.4}$$

Here we use a specific representation of the admissible domains Ω, or, in other words, of the admissible surfaces Γ.

Notations.

Γ_0 = reference surface, $\Gamma_0 \subset \text{int } \Phi$, $\partial\Gamma_0 \subset \partial\Phi$

$Z: \Gamma_0 \to \mathfrak{R}^3$ = fixed vector field on Γ_0 with

(a) Z is directed outwards with respect to Ω on $\text{int}(\Gamma_0)$

(b) Z is tangential to $\partial\Phi$ on $\partial\Gamma_0$

$A = \{u : \Gamma_0 \to \mathfrak{R} : u \text{ smooth}\}$ = space of variations of Γ_0.

Now the surfaces Γ taken into consideration have the form

$$\Gamma(u) = \{X = Y + u(Y)\, Z(Y) : Y \in \Gamma_0\}. \tag{2.5}$$

From now on, to clarify the relationships, we write

$$S(u),\ G(u),\ F(u),\ V(u), \text{ and } E(u)$$

and reformulate the variational problem (2.3) as

$$E(u^*) = \min\{E(u) : u \in A,\ V(u) = V_0\}. \tag{2.6}$$

Introducing the Lagrange functional

$$\begin{aligned} L(u) &= E(u) - \lambda(V(u) - V_0) \\ &= S(u) + bG(u) + \beta F(u) - \lambda(V(u) - V_0) \end{aligned} \tag{2.7}$$

with the Lagrange parameter λ we arrive at the Euler–Lagrange equation for problem (2.6), namely,

$$\langle \partial L(u), v \rangle = 0 \qquad \text{for all} \quad v \in A. \tag{2.8}$$

Using standard methods from differential geometry (cf. [6, 11]) we calculate

$$\partial L(u) = \partial S(u) + b\partial G(u) + \beta\partial F(u) - \lambda\partial V(u) \tag{2.9}$$

from

$$\langle \partial S(u), v\rangle = \int_\Gamma \frac{1}{\sqrt{g}}((v \wedge \partial_1 X)\cdot\partial_2(vZ) - (v\wedge\partial_2 X)\cdot\partial_1(vZ))\,d\Gamma, \tag{2.10a}$$

$$\langle \partial G(u), v\rangle = \int_\Gamma x_3 v\cdot Zv\,d\Gamma, \tag{2.10b}$$

$$\langle \partial F(u), v\rangle = \int_{\partial\Gamma} |Z\wedge\tau|\,v d(\partial\Gamma), \tag{2.10c}$$

$$\langle \partial V(u), v\rangle = \int_\Gamma v\cdot Zv\,d\Gamma. \tag{2.10d}$$

Here we have used the following symbols:

∂_i = derivatives with respect to the parameters of Γ

$\cdot,\ \wedge$ = scalar and vector product, respectively

$g = \det(\partial_i X\cdot\partial_j X)_{i,j=1,2} = |\partial X_1\wedge\partial X_2|^2$

$\nu = \dfrac{\partial X_1\wedge\partial X_2}{|\partial X_1\wedge\partial X_2|}$ = unit normal vector on Γ

τ = unit tangent vector on $\partial\Gamma$.

Remark. Integrating the differential of S by parts on Γ, one obtains

$$\langle \partial S(u), v\rangle = \int_\Gamma Mv\,d\Gamma + \int_{\partial\Gamma} v\cdot(Z\wedge\tau)\,v d(\partial\Gamma)$$

with

$$M = \frac{1}{\sqrt{g}}(\partial_1\nu\wedge\partial_2 X - \partial_2\nu\wedge\partial_1 X)\cdot Z$$
$$= \frac{1}{\sqrt{g}}(\partial_1\nu\cdot(\partial_2 X\wedge Z) - \partial_2\nu\cdot(\partial_1 X\wedge Z)).$$

Therefore, (2.8) is equivalent to

$$M + (bx_3 - \lambda)\,\nu\cdot Z = 0 \qquad \text{on} \quad \Gamma \tag{2.11a}$$

and

$$\nu\cdot(Z\wedge\tau) + \beta|Z\wedge\tau| = 0 \qquad \text{on} \quad \partial\Gamma \tag{2.11b}$$

If Z were equal to ν, we would obtain $\nu \cdot Z = 1$ and $M = -2H$ (H = mean curvature of Γ, see [6, p. 47]); hence (2.11a) means

$$2H = bx_3 - \lambda \qquad \text{on} \quad \Gamma. \tag{2.12a}$$

On the other hand, we have assumed that Z is tangential to $\partial\Phi$ on $\partial\Gamma$; since τ is also tangential to $\partial\Phi$, $Z \wedge \tau$ is normal to $\partial\Phi$. Therefore we obtain

$$\nu \cdot (Z \wedge \tau) = \cos\theta |Z \wedge \tau| \qquad \text{with } \theta = \text{angle between } \Gamma \text{ and } \Sigma;$$

hence (2.11b) means

$$\beta = -\cos\theta. \tag{2.12b}$$

3. The Finite Element Method

The numerical method used in this paper is a finite element method in the spirit of the orthodox Rayleigh–Ritz approach:

(a) We assume that Γ_0 is the union of triangles in $\mathfrak{R}^3$, which have n different vertices V_i, $i = 1, ..., n$. We call Γ_0 the "skeleton."

(b) To each vertex V_i we assign a direction $\hat{Z}_i \in \mathfrak{R}^3$, satisfying the same conditions as Z in 2. We construct a "chapeau" function $Z_i: \Gamma_0 \to \mathfrak{R}^3$ such that Z_i is continuous on Γ_0, linear on each triangle of Γ_0, and it satisfies

$$Z_i(V_j) = \hat{Z}_i \delta_{ij}, \qquad i, j = 1, ..., n,$$

δ_{ij} being the Kronecker symbol.

(c) The admissible surfaces are of the form

$$\Gamma(u) = \left\{ X = Y + \sum_{i=1}^{n} u_i Z_i(Y) : Y \in \Gamma_0 \right\}, \tag{3.1}$$

where u is the vector $(u_1, ..., u_n)$ of unknowns u_i. In this way, we get (3.1) by replacing

$$u(Y)\, Z(Y) \text{ in (2.5) by } \sum_{i=1}^{n} u_i Z_i(Y_i).$$

Following this procedure we obtain a family of surfaces in space all of which are unions of triangles; and each surface is represented by n unknowns u_i.

With the definitions (2.1), (2.2), and (2.4) for $E(u)$, $S(u)$, $G(u)$, $F(u)$, and $V(u)$, we now consider the discretized variational problem

$$E(u^*) = \min\{E(u) : u \in \mathfrak{R}^3,\ V(u) = V_0\}. \tag{3.2}$$

The Euler–Lagrange equation associated to this problem is

$$\frac{\partial}{\partial u_i} L(u) = 0 \qquad \text{for} \quad i = 1, \ldots, n. \tag{3.3}$$

with $L(u)$ defined by (2.7). Similarly to (2.10a)–(2.10d), the partial derivatives are given by

$$\frac{\partial}{\partial u_i} S(u) = \int_\Gamma \frac{1}{\sqrt{g}} ((v \wedge \partial_1 X) \cdot \partial_2 Z_i - (v \wedge \partial_2 X) \cdot \partial_1 Z_i)\, d\Gamma \tag{3.4a}$$

$$\frac{\partial}{\partial u_i} G(u) = \int_\Gamma x_3 v \cdot Z_i \, d\Gamma \tag{3.4b}$$

$$\frac{\partial}{\partial u_i} F(u) = \int_{\partial\Gamma} |Z_i \wedge \tau| \, d(\partial\Gamma) \tag{3.4c}$$

$$\frac{\partial}{\partial u_i} V(u) = \int_\Gamma v \cdot Z_i \, d\Gamma. \tag{3.4d}$$

The integrals involved are evaluated separately for each triangle that is adjacent to the vertex V_i and then the contributions are summed up to give the derivative.

In principle, if the volume V_0 is prescribed the Lagrange parameter λ is an unknown to be determined as part of the problem. For this mathematical study, we have decided to prescribe λ and obtain a certain volume V. In a future paper we are going to investigate in more detail the relationship between V and λ; cf. also [5].

Naturally, (3.3) is a nonlinear system of equations for the unknowns u_i, $i = 1, \ldots, n$. This is solved by the classical Newton method, i.e., the second derivatives of $L(u)$ are calculated explicitly. The linear system to be solved in each iteration step has a sparse symmetric indefinite matrix. This is dealt with using a variant of the conjugate gradient algorithm developed in [10]. The major advantage of this approach is that no matrix has to be stored, but only a procedure has to be provided which calculates the product of the matrix multiplied with a vector.

4. Details of the Algorithm

The realization of the finite element method used in this paper has the following steps:

Step 1. The skeleton, i.e., the triangles that Γ_0 consists of, is obtained by successive refinements of a coarse skeleton. One starts with a small number of triangles, e.g., 1, 2, or 3 and refines recursively in a regular way. The data sets needed to store the necessary information contain

— a list of triangles with their edges and vertices,

— a list of edges belonging to $\partial\Gamma$,

— a list of coordinates of the vertices,

— a list of coordinates of the directions $\hat{Z}_i$ at the vertices V_i.

Step 2. In each refinement step the directions $\hat{Z}_i$ are interpolated linearly; thus the basic properties required of Z are maintained.

Step 3. Since Newton's method has safe convergence properties only if the initial guess is close enough to the solution, the following homotopy strategy is applied: initially, a skeleton is constructed according to (a). Then this skeleton is modified in the directions $\hat{Z}_i$ such that it approximates a sphere with given centre and radius r or cylinder with given axis and radius. This sphere, or cylinder, resp., solves (2.12a) with $b=0$ and $\lambda=2/r$, or $\lambda=1/r$, respectively; it intersects the walls $\partial\Phi$ with known angles θ, not necessarily the same everywhere. Therefore this skeleton solves (3.3) approximately with known parameters; the residual is smaller the finer the triangulation is chosen.

Step 4. The Bond number and the angles are modified in small steps in the sense of a continuation method until the problem in question is reached. During the process of this homotopy, the skeleton is updated whenever a solution is found; i.e., the old solution X of the form (3.1) is used as the new skeleton Γ_0 for the next Newton iteration.

Step 5. After reaching the target values of the continuation process, one or more additional refinements may be carried out and followed by another cycle of Newton iterations to obtain a highly accurate solution on a fine grid.

5. Results

The method described in this paper was used to solve the problem of determining the shape of capillary surfaces in the following cases:

(a) A sessile drop: $\Phi=\{x:x_3>0\}$, see Fig. 5.1.

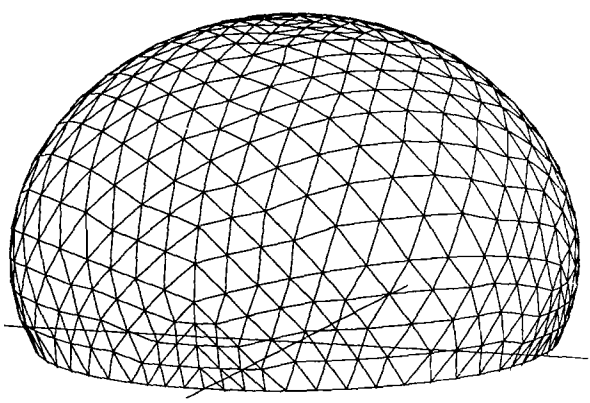

FIG. 5.1. The sessile drop: $b=1$, $\theta=120°$, $V_0=2.04$, $S=6.34$, $\lambda=3$.

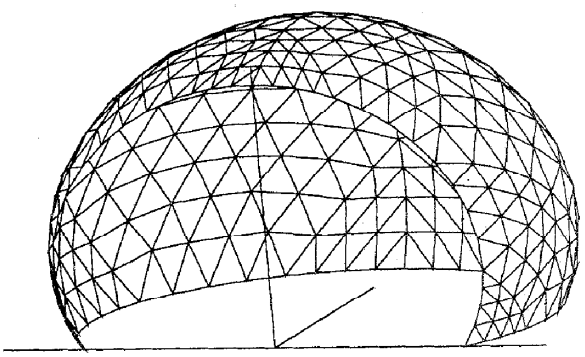

FIG. 5.2. The drop on an edge: $b=1$, $\theta=120°$, $V_0=1.73$, $S=4.72$, $\lambda=3$.

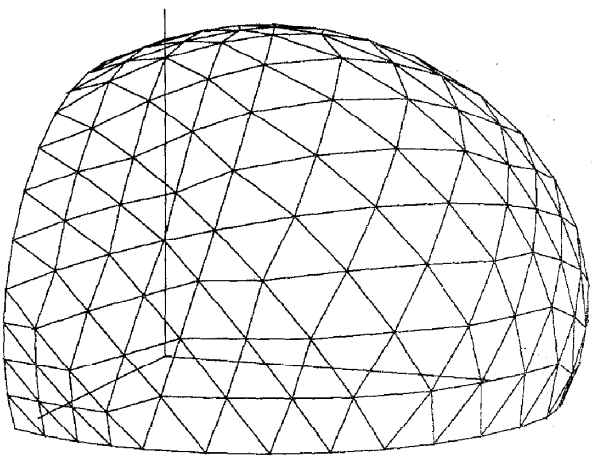

FIG. 5.3. The drop in a corner: $b=1$, $\theta=120°$, $V_0=1.44$, $S=3.4$, $\lambda=3$.

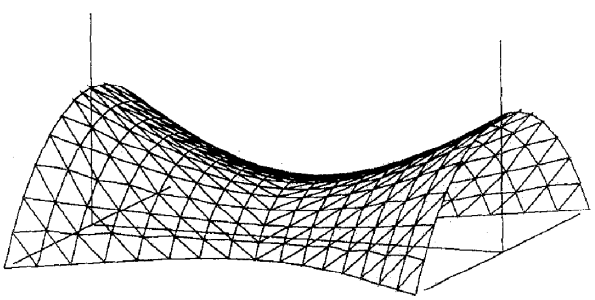

FIG. 5.4. The sessile drop between two parallel planes: $b=0$, $\theta=60°$, $V_0=0.95$, $S=4$, $\lambda=0.6$.

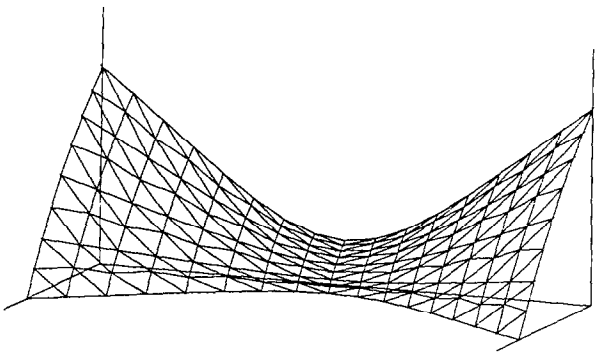

FIG. 5.5. The drop in a box: $b=0$, $\theta=60°$, $V_0=0.23$. $S=1.34$, $\lambda=0.33$.

(b) A drop on an edge: $\Phi=\{x: x_2>0, x_3>0\}$, see Fig. 5.2.

(c) A drop in a corner: $\Phi=\{x: x_1>0, x_2>0, x_3>0\}$, see Fig. 5.3.

(d) A sessile drop between two parallel planes: $\Phi=\{x: -1<x_1<1, x_3>0\}$, see Fig. 5.4.

(e) A drop in a box: $\Phi=\{x: -1<x_1<1, x_2>0, x_3>0\}$, see Fig. 5.5.

Case (a) was also solved as a boundary value problem for a system of ordinary differential equations. Due to the axial symmetries of the problem standard methods can be used for this [3]. The results rounded to two decimals are

$$\lambda=3.00, \qquad V=2.04, \qquad S=6.33.$$

This is in good agreement with the values obtained with the proposed finite element method, see Fig. 5.1.

5. PERFORMANCE

For all of the five examples presented in Section 4 we give in the following a detailed account of the computational procedure and its performance. For examples 1–3 and 4–5, respectively, we report which specific choices were made in the five steps of the algorithm as given in Section 4 and which computational work was involved.

EXAMPLES 1–3 In Step 1 one initial triangle is used and this (Step 2) is refined twice. Subsequently the vertices of the planar triangulated surface are projected radially onto a sphere of radius 2 with center

(0, 0, 1) for Example 1,

(0, 1, 1) for Example 2,

(1, 1, 1) for Example 3.

The resulting contact angle attained all along the intersection of the spherical surface and the walls is $\theta = 120°$. The number of points on the surface is 15. In Step 4 the parameters $b(\lambda)$ are simultaneously modified from 0(1) to 1(3), respectively, in five uniform homotopy steps. The number of Newton iterations in each of these steps is 3 or 4. The number of cg-iterations needed to solve the associated linear systems varies somewhat from step to step but is approximately

$$0.4N \quad \text{for} \quad \text{Example 1,}$$

$$0.7N \quad \text{for} \quad \text{Example 2,}$$

$$0.5N \quad \text{for} \quad \text{Example 3;}$$

here N denotes the number of unknowns u_i, cf. (3.1). The target values in b and λ are reached but the discretization is much too coarse. Thus, in Step 5 two more refinements are carried out with subsequent Newton corrections requiring 4 to 5 iterations and cg-iterations of $0.75N$, $0.3N$, and $0.75N$ for the three examples where now $N = 153$.

EXAMPLES 4–5. The initial triangulation consists of two triangles (Step 1) and it is refined twice (Step 2). Then the resulting vertices are moved (Step 3) to a cylinder of radius 1 and axis in the direction of (0, 0, 1) yielding a contact angle of 90° and 25 unknowns. The parameters $\theta(\lambda)$ are decreased in Step 4 to 60° and 0.6, 0.3 in Examples 4, 5, respectively. For this 3–4 Newton and $0.75N$ (resp. $0.7N$) cg-iterations are needed. Finally, one more refinements leads in Step 5 to 81 unknowns requiring 4 Newtons and $0.5N$ cg-iterations for the corrector.

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