Numerical Solutions for Intermediate Angles for the Laplace-Young Capillary Equations

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Numerical Solutions for Intermediate Angles of the Laplace-Young Capillary Equations

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Abstract

Capillarity is the phenomena of fluid rise against a solid vertical wall. In this paper, we consider bounded cases of intermediate corner angles $(\pi/2 < \alpha + \gamma < \pi/2 + 2\gamma)$, where γ is the angle of contact and 2α is the wedge angle. The Laplace-Young Capillary equations are used to determine the rise of the fluid, especially at corners. While there exist asymptotic expansions for the height rise occurring at the corner of an intermediate angle, not all coefficients are known analytically. Therefore, numerical solutions are necessary, even though only a few numerical methods have been published. We explain our least-squares finite element method used in determining solutions to the Laplace-Young Capillary equations, and then give our numerical results.

1   Introduction

The solutions of the Laplace-Young Capillary equations, $u(x, y)$, give the height rise of liquid at a given point in Cartesian coordinates (x, y) in the domain Ω. In terms of polar coordinates, $u(r, \theta)$ is equivalent to the height rise at a point (r, θ), with the conversion $x = r\cos\theta$, $y = r\sin\theta$. On domains containing a wedge angle, much attention has been given to developing asymptotic solutions to the height at the corner point [7], [9], $r = 0$. The angle 2α measures the wedge, where $\theta = 0$ bisects the wedge angle. The angle given by the contact of the liquid against the vertical wall is γ (see Figure 1). Corner angles are classified into three different categories: small, intermediate, and large; previously determined analytic solutions are given below for each case.

1) Small angles: $0 < \alpha < \pi/2 - \gamma$

As the solution for the small angles approaches the corner, the height rise, $u(r, \theta)$, is unbounded [5]:

$$u \sim \frac{\cos\theta - (a^2 - \sin^2\theta)^{1/2}}{ar} + O(r^3),$$

where $a = \sin\alpha/\cos\gamma$ and $\theta = \pm\alpha$.

2) Intermediate angles: $\pi/2 - \gamma < \alpha < \pi/2 + \gamma$

The analytic solutions that have been determined for intermediate angles are bounded and in the form of a power series expansion [5]:

$$u \sim u_0 - \frac{r\cos\theta}{(a^2 - 1)^{1/2}} + \cdots.$$

3) Large angles: $\pi/2 + \gamma < \alpha < \pi$

Height solutions for large angles remain bounded, but the slopes approaching $r = 0$ are not. An analytical solution to the large angles is not yet given and knowledge of the far field condition is required to determine u [7].
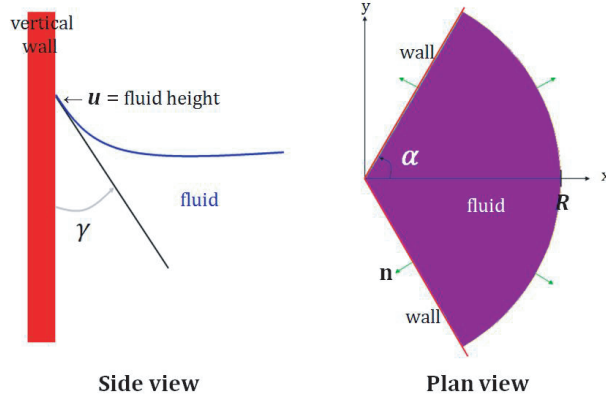
Figure 1: α and γ

2   Laplace-Young Capillary Equations and Analytical Solutions

Solving the Laplace-Young equations gives the height rise of fluid at a given point. These equations are as follows:

$$
\begin{cases}
\nabla \cdot \left(\dfrac{\nabla u}{\sqrt{1 + |\nabla u|^2}} \right) = \kappa u \;\; \text{in} \;\; \Omega \\[4mm]
\mathbf{n} \cdot \left(\dfrac{\nabla u}{\sqrt{1 + |\nabla u|^2}} \right) = \cos \gamma \;\; \text{on} \;\; \partial \Omega,
\end{cases}
\tag{1}
$$

where κ is the capillary constant of the liquid. $\kappa > 0$ indicates positive gravity, $\kappa < 0$ indicates negative gravity, and $\kappa = 0$ indicates zero-gravity scenario. The unit vector normal to the boundary $\partial \Omega$ is denoted by $\mathbf{n}$.

The focus in this paper is the intermediate corner angles, and the asymptotic power series solution for these bounded solutions is as follows:

$$
u(r, \theta) = u_0 + r u_1(\theta) + r^2 u_2(\theta) + r^3 u_3(\theta) + ... = \sum_{i=0}^{i} r^i u_i(\theta).
$$

Here, u_0 is given to be the height rise of the solution at $r = 0$ and $u_1(\theta) = \frac{cos\theta}{(a^2-1)^{1/2}}$, which determines the slope to the solution as $r \to 0$ and $\theta = \pm\alpha$. The coefficients of this power series, $u_i(\theta)$, are known in terms of u_0. However, since u_0 is not known analytically, the only coefficient truly known is $u_1(\theta)$ because it does not depend on θ. Thus, once u_0 is determined, the remainder of the power series solution is known analytically[8]. Note that this power series is the same solution given in the introduction.

3   Numerical Methods

3.1   Rescaling Laplace-Young

In solving the Laplace-Young equations, a rescaling of the equations to capillary unit lengths (κ) simplifies the problem. Taking the original form of the Laplace-Young equations with a solution of u_{old}, and making

a substitution of $u_{old} = Lu_{new}$, where $L = 1/\kappa$, (1) becomes the following equations:

$$\begin{cases} \nabla \cdot \left(\dfrac{\nabla Lu_{new}}{\sqrt{1 + |\nabla Lu_{new}|^2}} \right) = \kappa Lu_{new} \ \ \text{in} \ \ \Omega \\ \mathbf{n} \cdot \left(\dfrac{\nabla Lu_{new}}{\sqrt{1 + |\nabla Lu_{new}|^2}} \right) = \cos\gamma \ \ \text{on} \ \ \partial\Omega. \end{cases} \tag{2}$$

Where ∇Lu_{new} occurs, the substitution (in Cartesian coordinates) $x_{old} = Lx_{new}$ and $y_{old} = Ly_{new}$ is used, noting that L is a constant:

$$\nabla Lu = \begin{pmatrix} Lu_x \\ Lu_y \end{pmatrix} = \begin{pmatrix} \partial Lu/\partial Lx \\ \partial Lu/\partial Ly \end{pmatrix} = \begin{pmatrix} u_x \\ u_y \end{pmatrix} = \nabla u.$$

It follows that $\nabla Lu_{new} = \nabla u_{new}$ and (1) becomes the rescaled Laplace-Young equation:

$$\begin{cases} \nabla \cdot \left(\dfrac{\nabla u}{\sqrt{1 + |\nabla u|^2}} \right) = u \ \ \text{in} \ \ \Omega \\ \mathbf{n} \cdot \left(\dfrac{\nabla u}{\sqrt{1 + |\nabla u|^2}} \right) = \cos\gamma \ \ \text{on} \ \ \partial\Omega. \end{cases} \tag{3}$$

The scale for the solutions on Ω is now given in capillary length units, and this form of the Laplace-Young equations will be used throughout the rest of the paper.

3.2   Linearization

Since (3) has nonlinear terms associated with it, a linearization of the equations will be done with a current approximation of the unknown, such that
$$b \approx u.$$

An initial value of b must be assigned, and $b = 0$ works as a first approximation. Now, we consider the series of linear problems from

$$\begin{cases} \nabla \cdot \left(\dfrac{\nabla u}{\sqrt{1 + |\nabla b|^2}} \right) = u \ \ \text{in} \ \ \Omega \\ \mathbf{n} \cdot \left(\dfrac{\nabla u}{\sqrt{1 + |\nabla b|^2}} \right) = \cos\gamma \ \ \text{on} \ \ \partial\Omega. \end{cases} \tag{4}$$

For simplification of notation, let

$$A = A(\nabla b) = \frac{1}{\sqrt{1 + |\nabla b|^2}},$$

and $A(\nabla b)$ will be the known approximation of the nonlinear system. The system can then be written as

$$\begin{cases} \nabla \cdot (A\nabla u) - u = 0 \\ \mathbf{n} \cdot (A\nabla u) - cos\gamma = 0. \end{cases} \tag{5}$$

Using the product rule and the property $\nabla \cdot (\nabla) = \Delta$, (5) becomes

$$\begin{cases} A\Delta u + \nabla A \cdot \nabla u - u = 0 \\ \mathbf{n} \cdot (A\nabla u) - cos\gamma = 0. \end{cases}$$

3

In addition to these equations, define $U = \nabla u$ as a new unknown to approximate. Also true is that $\nabla \times \nabla = 0$, and therefore another equation can be added: $\nabla \times U = 0$ in the domain Ω. Combining all equations, the PDE system now looks like

$$\begin{cases} A\nabla \cdot U + \nabla A \cdot U - u = 0 \\ \qquad\qquad\qquad \nabla \times U = 0 \quad \text{in} \quad \Omega \\ \qquad\qquad \nabla u - U = 0, \end{cases} \tag{6}$$

with a boundary condition of

$$\mathbf{n} \cdot (AU) - cos\gamma = 0 \quad \text{on} \quad \partial\Omega.$$

With $A = A(\nabla b)$, the system is now linear.

3.3 Least-Squares Finite Element

We seek to find a solution to (6) by the least-squares finite element approach. To do this we define the following least-squares functional:

$$G(U, u) = ||A\nabla \cdot U + \nabla A \cdot U - u||^2 + ||\nabla \times U||^2 + ||\nabla u - U||^2,$$

for all $u \in \mathbf{V} = \{v \in H^1(\Omega) : \mathbf{n} \cdot \nabla v = \cos \gamma\}$ and $U \in \mathbf{U} = \{V \in H^1(\Omega) : \mathbf{n} \cdot V = \cos \gamma\}$. Minimizing $G(U, u)$ over $\mathbf{U} \times \mathbf{V}$ yields a symmetric positive definite variational problem. When $\mathbf{U}$ and $\mathbf{V}$ are replaced with appropriate finite element spaces, the problem becomes a large positive definite system of algebraic equations which can be solved efficiently. For more details on the least-squares finite element approach, please see [3].

We thus solve a sequence of linear problems of the form (6), where each iteration takes $b = u_{old}$ and $u = u_{new}$. As we iterate, the solution tends toward that of (3), the original nonlinear problem.

4 Convergence of Solutions

4.1 Sobolev Spaces

We begin our discussion of convergence by defining our notation for Sobolev Spaces [1]. Let $W^{k,p}(\Omega)$ denote the standard Sobolev Space defined by integers k and p, where

$$u \in W^{k,p} \Leftrightarrow (\sum_{|\alpha| \leq k} |D^\alpha u|^p)^{1/p} \equiv ||u||_{k,p} < \infty.$$

When $p = 2$, we simplify the notation by introducing the spaces

$$H^k(\Omega) = W^{k,2}(\Omega),$$

and use the norm $|| \cdot ||_k = || \cdot ||_{k,2}$.

Consider an illustration of this notation in the one dimensional case: If a single-variable function is contained in the Sobolev Space $H^0(\Omega)$, the following condition holds:

$$\int_0^1 f(t)^2 dt < \infty.$$

To be contained in the Sobolev space $H^1(\Omega)$, a function, f, and its first derivative, f', must be bounded in the interval $[0, 1]$:

$$\int_0^1 (f(t)^2 + f'(t)^2)dt < \infty.$$

And likewise, this can be generalized such that if a function is contained in the Sobolev Space $H^n(\Omega)$ if

$$\int_0^1 (f(t)^2 + f'(t)^2 + \ldots + f^{(n)}(t)^2)dt < \infty.$$

With these definitions, it can be seen that the Sobolev Spaces embed into each other. When a function is contained in $H^2(\Omega)$ for example, it is also contained in $H^1(\Omega)$ and $H^0(\Omega)$. Similar definitions hold for the multi-variable case that we present.

4.2   Convergence of the Least-Squares Solution

Now, convergence of the least-squares solution is consistent with the convergence of the functional. Previous results from Cai et al [3] have been given to confirm functional convergence, and showing that the given method fits into the case outlined will prove the convergence of the solutions. To begin, the form of the problem must be given as follows:

$$\begin{cases} \nabla \cdot (A\nabla u) - u = f & \text{in } \Omega \\ \mathbf{n} \cdot A\nabla u = 0 & \text{on } \delta\Omega. \end{cases}$$

Therefore, the Laplace-Young equations must be modified into this form. To do so, take the original system:

$$\begin{cases} \nabla \cdot A\nabla \tilde{u} - \tilde{u} = 0 & \text{in } \Omega \\ \mathbf{n} \cdot A\nabla \tilde{u} = cos\gamma & \text{on } \delta\Omega \end{cases} \tag{7}$$

and consider the related problem

$$\begin{cases} \Delta u_0 = 0 & \text{in } \Omega \\ \mathbf{n} \cdot A\nabla u_0 = cos\gamma & \text{on } \delta\Omega, \end{cases} \tag{8}$$

which has a solution $u \in H^k(\Omega)$ that is unique up to a constant, where $k < \pi/2 + 1$. [4]. And from this, (7) similarly has a solution $\tilde{u} \in H^k(\Omega)$. Note: α can be chosen sufficiently small in order to find a sufficiently large k.

Let $u = u_0 - \tilde{u}$, then

$$\nabla \cdot A\nabla u - u = \nabla \cdot A\nabla(u_0 - \tilde{u}) - (u_0 - \tilde{u})$$
$$= \nabla \cdot A\nabla u_0 - u_0$$
$$\equiv f.$$

Notice that $f \in H^{k-2}(\Omega)$ since there are two derivatives of u. And on $\delta\Omega$,

$$\mathbf{n} \cdot A\nabla u = \mathbf{n} \cdot A\nabla u_0 - \mathbf{n} \cdot A\nabla \tilde{u} = 0.$$

Combining these two equations, a system matching the required form is created:

$$\begin{cases} \nabla \cdot (A\nabla u) - u = f & \text{in } \Omega \\ \mathbf{n} \cdot A\nabla u = 0 & \text{on } \delta\Omega. \end{cases} \tag{9}$$

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Now that the system given has the correct form, assumptions about the problem must be satisfied[3].

Assumption A_0: $\int_\Omega u = 0$ so that a Poincare inequality holds. It is known that $\tilde{u}$ satisfies $\int \tilde{u} = 0$, and we may choose $u_0 \in H^k(\Omega)/\mathbb{R}$ so that $\int u = 0$ as well.

Assumption A_1: Ω is bounded, open, connected, convex, and piecewise $C^{1,1}$. We consider only such domains.

Assumption A_2: The boundary of Ω is composed of Dirichlet and Neumann parts. The boundary conditions in equation (9) are of Neumann type.

Assumption A_3: A is $C^{1,1}$.

Recall the linearized form of the Laplace-Young equations:

$$\begin{cases} A(\nabla b)\nabla \cdot U + \nabla A(\nabla b) \cdot U - u = 0 \\ \mathbf{n} \cdot (A(\nabla b)U) - cos\gamma = 0, \end{cases} \tag{10}$$

where $A(\nabla b) = \frac{1}{\sqrt{1+|\nabla b|^2}}$ and $b \approx u$ is the old solution used to linearize the system.

A Sobolev space embeds into a continuous space in $\mathbb{R}^n$ under the following conditions from [4]

$$W^{m,p}(\Omega) \hookrightarrow C^{0,1}(\overline{\Omega}),$$

where

a) $m \geq 0$ and $1 \leq p \leq \infty$ where m and p are integers,

b) $\frac{n}{p} + 1 < m$,

c) Ω is open, connected, Lipschitz boundary.

Therefore,

$$\text{if } u \in W^{m+j,p}(\Omega), \text{ then } \sum_{|\alpha| \leq j} |D^\alpha u| \in W^{m,p}(\Omega) \hookrightarrow C^{0,0}(\overline{\Omega}),$$

which means that $u \in C^{j,1}(\overline{\Omega})$ for any $j \in \mathbb{N}$.

More specifically, for the Laplace-Young equations, $n = 2$, $p = 2$, and $j = 1$. Choose some $\delta > 0$, so that when $\nabla b \in H^{m+1}(\Omega)$, it embeds into $C^{1,1}(\overline{\Omega})$ for $m = 2 + \delta$. Thus,

$$b \in H^{4+\delta}(\Omega) \Rightarrow \nabla b \in H^{3+\delta}(\Omega) \hookrightarrow C^{1,1}(\overline{\Omega}).$$

Lemma 4.1 *Let* $A(f) = \frac{1}{\sqrt{1+|f|^2}}$. *If* $f \in C^{1,1}(\overline{\Omega})$, *then* $A(f) \in C^{1,1}(\overline{\Omega})$.

Proof. Since $f \in C^{1,1}(\overline{\Omega})$ for a given f, then $\nabla f \in C^{0,1}(\overline{\Omega})$. Thus, it must be shown that $A(f)$ and $\nabla A(f)$ are contained in $C^{0,1}(\overline{\Omega})$. Since the function A is continuous, and the composition of continuous functions is also continuous, then it follows that $A(f) \in C^{0,1}(\overline{\Omega})$. Now, $\nabla A(f) = \frac{-f\nabla f}{(1+f^2)^{3/2}}$, which is also a composition of continuous functions, and therefore also continuous and in $C^{0,1}(\overline{\Omega})$. ∎

Note: $u_0 \in H^k(\Omega) = H^{4+\delta}(\Omega)$ for $4 + \delta < \frac{\pi}{2\alpha} + 1$. Solving for the domain angle, $\alpha < \frac{\pi}{2(3+\delta)}$. Therefore, a choice of $\alpha < \frac{\pi}{6}$ if $\delta \in \mathbb{R}$ or $\alpha < \frac{\pi}{8}$ if $\delta \in \mathbb{N}$.

Let T_h be a regular triangulation of the domain, Ω, and assume there exist two finite element approximation subspaces defined over T_h:

$$\mathbf{U}_h \subset \mathbf{U} \text{ and } \mathbf{V}_h \subset \mathbf{V}.$$

The finite element approximation to the problem is determining $(U_h, u_h) \in \mathbf{U}_h \times \mathbf{V}_h$ such that

$$G(U_h, u_h) \leq G(V_h, v_h) \ \ \forall \ (V_h, v_h) \in \mathbf{U}_h \times \mathbf{V}_h. \tag{11}$$

$\mathbf{U}_h$ and $\mathbf{V}_h$ are defined as piecewise linear finite element spaces:

$$\mathbf{V}_h = \{v \in C^0(\Omega) : q|k \in P_1(K) \ \ \forall \ K \in T_h, v \in \mathbf{V}\}$$

and

$$\mathbf{U}_h = \{V \in C^0(\Omega)^n : v_l|k \in P_1(K) \ \ \forall \ K \in T_h, V \in \mathbf{U}\},$$

where $P_1(\mathrm{K})$ is the space containing polynomials with degree no more than one. Note that extending the results is easy to show for finite element approximations with higher-order.

Theorem 4.2 *Given the form of the problem and $A_0 - A_3$. Assume that the solutions (U, u) of (9) are contained in $H^{1+\delta}(\Omega)^{n+1}$ for some $\delta \in [0, 1]$. Let $(U_h, u_h) \in \mathbf{U}_h \times \mathbf{V}_h$ be the solution of (11). Then,*

$$\|u - u_h\|_{1,\Omega} + \|U - U_h\|_{1,\Omega} \leq Ch^\delta(\|u\|_{(1+\delta),\Omega} + \|U\|_{(1+\delta),\Omega}),$$

where C does not depend on h, u, or U.

Proof. Using the results of the assumptions given and showing the form of the problem matches, the proof follows directly from [3].

Therefore, functional convergence of the solution works to confirm the convergence to the correct desired solution of the Laplace-Young equations.

5 Numerical Results

Numerical results are given for intermediate angles and the domain used in computation is defined as:

$$\Omega = \{(r, \theta); 0 < r < R, -\alpha < \theta < \alpha\}.$$

Table 1 demonstrates the convergence of the numerical slope to analytical solutions. As the discretization, T_h, of the domain is further refined with increasing values of n, the slope of the solution becomes arbitrarily close to the analytical solution. If h is defined as the width of each triangle along $\partial\Omega$ in T_h, then $n = 1/h$. Near the corner, a finer discretization is used with $2n$ divisions, and further away there are only n divisions so that there is more focus near $r = 0$. An illustration of the triangulation of Ω is given in Figure 2 for a value of $n = 16$.

Table 1 shows this trend in the case where $\alpha = \pi/3$ and $\gamma = \pi/4$. Recall that the slope of the solution as $r \to 0$ is given in the power series solution by

$$u_1 = \frac{cos\theta}{(a^2 - 1)^{1/2}},$$

and for our specific case, $\theta = \alpha = \pi/3$ and $\gamma = \pi/4$. Therefore, the desired analytical slope is $u_1 = \sqrt{2}/2 \approx 0.707107$. Table 1 shows the error in the slope is reduced approximately linearly, giving confidence in the method and our approximation to u_0.
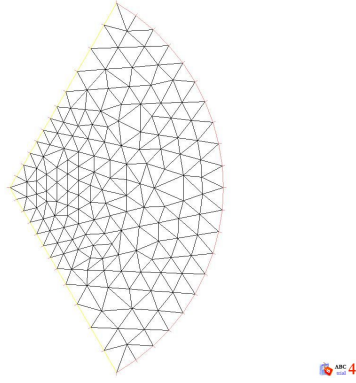
Figure 2: Triangulation of Ω, $n = 16$

n	slope	error in slope	height
8	-0.568429	0.138678	1.25086
16	-0.652611	0.054496	1.2375
32	-0.693487	0.013620	1.22373
64	-0.701674	0.005433	1.21642
128	-0.703394	0.003713	1.2145
$\vdots$	$\vdots$	$\vdots$	$\vdots$
∞	$\sqrt{2}/2 \approx 0.707107$	0.0	unknown

Table 1: Slope Convergence: $\alpha = \pi/3$ and $\gamma = \pi/4$

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γ	$\alpha = \pi/3$	$\alpha = \pi/4$
40	1.3692	n/a
45	1.2145	n/a
50	1.0683	1.54862
55	0.928488	1.30146
60	0.792122	1.08994
65	0.65801	0.894685
70	0.525264	0.708507
75	0.393391	0.527729
80	0.262018	0.350248
85	0.130943	0.174659

Table 2: Heights: $n = 128$

In Table 2, various combinations of α and γ are given, along with the numerical results for their heights. In all cases, $n = 128$ and similar analysis of the convergence of the numerical slopes to the analytical slopes was confirmed.

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