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体積保存条件を伴う双曲型自由境界問題の数値シミュレーション
Numerical simulation to the hyperbolic free boundary problem with volume constraint

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Abstract. The motion of a bubble on water surface is investigated numerically. The bubble is described by using a graph of scalar function. The bubble moves on the water surface while changing shape, but its volume is always preserved. The edge of bubble is called a free boundary, therefore, the problem becomes a free boundary problem of degenerate hyperbolic type with volume constraint. A minimizing method via the discrete Morse flow of hyperbolic type works well numerically to this problem.

1 Introduction

In this paper, we treat a motion of bubble which moves on water surface while changing its shape numerically. We use the graph of a scalar function u to describe the shape of the bubble. The zero level set of u coincides with the water surface. The set of points where the bubble touches the water surface is called *free boundary*. In order to simplify the model, we assume that the water layer is so thin that its flow or movement does not influence the bubble. Moreover, water density σ is expected to be constant, and the stress tensor density of the bubble and water surface T to be homogeneous and isotropic.

We also assume that the volume of air which is surrounded by the bubble is preserved at any time, that is, the bubble movement can be described by wave equation with volume constraint (i.e., $\int_\Omega u dx = M$). The following equation describes the phenomena well:

$$\chi_{u>0}\, u_{tt} = \Delta u - Q^2(\chi^\varepsilon)'(u) + \lambda\chi_{u>0}. \tag{1.1}$$

Here $\chi_{u>0}$ is the characteristic function of the set $\{u > 0\}$ and $\chi^\varepsilon \in C^2(\mathbf{R})$ is a smoothing of χ satisfying

$$\chi^\varepsilon(s) = \begin{cases} 0, & s \leq 0 \\ 1, & \varepsilon \leq s \end{cases}$$

with interpolating in $0 < s < \varepsilon$ in such a way that $|(\chi^\varepsilon)'(s)| \leq C/\varepsilon$ and $\int_0^\varepsilon (\chi^\varepsilon)'(s)\, ds = 1$. The term $(\chi^\varepsilon)'(u)$ describes the adhesive force which generates new surface against surface tension of water while moving the free boundary. It is due to this term that oscillation of solution in the whole domain does not occur.

The specificity of this equation lies in the coefficient $\chi_{u>0}$ on the left-hand side. Because of this coefficient, non-negativity of the solution is guaranteed. We will show how to get above equation.

1.1 Energy conserving case

When the energy of bubble system is conserved, the Lagrangian of bubble system is calculated as follows:

$$\mathcal{L} = \frac{1}{2}\int_\Omega \left(T\left|\nabla u\right|^2 + \widetilde{Q}^2\chi_{u>0} - \sigma\left(u_t\right)^2\chi_{u>0} \right) dx. \tag{1.2}$$

Here Ω is a domain in $\mathbf{R}^m$ and $\widetilde{Q} > 0$ is a adhesion. The term $\sigma\left(u_t\right)^2\chi_{u>0}$ describes the velocity energy density of bubble to the vertical direction and $T\left|\nabla u\right|^2 + \widetilde{Q}^2\chi_{u>0}$ describes the potential energy coming from the shape of bubble. The feature of $\mathcal{L}$ is that the velocity energy disappears when the film of bubble goes under the water surface.

The action integral is defined by $J\left(u\right) = \int_0^\tau \mathcal{L}\,dt$ and the problem is to find a stationary point of the functional J in the suitable function space satisfying volume constraint. At the first, let us set test function $u^\delta = \frac{u+\delta\zeta}{\int_\Omega (u+\delta\zeta)\,dx}$, $\zeta \in C_0^\infty\left(\Omega_\tau \cap \{u>0\}\right)$ and take the first variation of J:

$$u_{tt} = \Delta u + \lambda \quad (x,t) \in \Omega_\tau \cap \{u > 0\}.$$

Without loss of generality, we choose all constants such as stress tensor density T, mass density of the film σ or volume of bubble M to be the simplest one ($T = \sigma = M = 1$). And we denote by $Q = \widetilde{Q}/T$, $\Omega_\tau = \Omega \times (0,\tau)$.

In order to get the free boundary condition, let us set test function $v^\delta = \frac{u\left(\varphi^{-1}(z')\right)}{\int_\Omega u(\varphi^{-1}(z'))\,dx'}$, $z' = (x',t') = \varphi\left(z\right) = z + \delta\eta\left(z\right)$, $\eta \in C_0^\infty\left(\Omega_\tau, \mathbf{R}^{\mathbf{M}+1}\right)$ and take the inner variation of J:

$$\left|\Delta u\right|^2 - \left(u_t\right)^2 = Q^2 \quad (x,t) \in \Omega_\tau \cap \partial\{u > 0\},$$

here we denote $z = (x,t)$.

We obtain the explicit form of the Lagrange multiplier λ as

$$\lambda = \int_\Omega \left(\left|\nabla u\right|^2 + u u_{tt}\,\chi_{u>0} \right) dx. \tag{1.3}$$

The integral representation of Lagrange multiplier makes the problem more difficult. However, we can calculate an approximate solution to (1.1) by use of a time-semidiscretized functional which is called *the discrete Morse flow of hyperbolic type* (see [7]).

1.2 Energy loosing case

On the other hand, when a part of the film which composes the bubble goes down under the water surface, the energy of bubble system is not preserved. In this case, if one consider the equation $v_{tt} = \Delta v + Q^2 (\chi^\varepsilon)'(v)$, $u = \max(v, 0)$ is expected to be a solution to this phenomena. In such a case, the free boundary condition is not expected to be satisfied. But such solutions are still satisfy the equation (1.1).

2 Free Boundary Condition

In this section, we formally derive free boundary condition for the free boundary problem which is obtained when ε is taken to zero in (1.1).

Proposition 2.1. *If we assume the existence of u^ε, the classical solution to (1.1), and $u^\varepsilon \longrightarrow \exists v$ $(\varepsilon \to 0)$ in some suitable sense (assumptions are shown in the calculation) with v satisfying $\Delta v - v_{tt} = \lambda$ in $\Omega_T \cap \{v > 0\}$, then the equality $|\nabla v|^2 - (v_t)^2 = Q^2$ on $\partial\{v > 0\}$ holds.*

Proof. To show this, we multiply $\zeta u_k^\varepsilon \left(\equiv \zeta \frac{\partial u^\varepsilon}{\partial x_k}\right)$ to both sides of (1.1) and integrate on Ω_T, $(\zeta \in C_0^\infty(\Omega_T))$. We get the following identity (see [2]):

$$\int_{\Omega_T} \zeta u_k^\varepsilon \left(\Delta u^\varepsilon - \chi_{u^\varepsilon>0} u_{tt}^\varepsilon - \lambda^\varepsilon \chi_{u^\varepsilon>0}\right) dz = \int_{\Omega_T} Q^2 \zeta u_k^\varepsilon (\chi^\varepsilon)'(u^\varepsilon) dz. \tag{2.1}$$

Noting that $[\chi^\varepsilon(u)]_{x_k} = (\chi^\varepsilon)'(u)\, u_k$ and by the integration by parts, the right-hand side of (2.1) can be calculated in the following way:

$$\begin{aligned}
(\text{r.h.s.}(2.1)) &= -\int_{\Omega_T} Q^2 \zeta_k \chi^\varepsilon(u^\varepsilon) dz \\
&\xrightarrow[\varepsilon \to 0]{} -\int_{\Omega_T \cap \{v>0\}} \zeta_k Q^2 dz \quad (u^\varepsilon \to v,\ \chi^\varepsilon(u^\varepsilon) \to \chi_{v>0} \text{ are assumed}) \\
&= -\int_{\Omega_T \cap \partial\{v>0\}} \zeta Q^2 \nu_k dS,
\end{aligned}$$

where ν_k is the k-th element of the outer normal $\nu = (\nu_1 \cdots \nu_{n+1})$ to the set $\{v > 0\} \subset \Omega_T$ with ν_{n+1} being the t direction.

On the other hand, the left-hand side of (2.1) can be calculated as follows:

$$
\begin{aligned}
(\text{l.h.s.}(2.1)) &= -\int_{\Omega_T} [\nabla(\zeta u_k^\varepsilon)\nabla u^\varepsilon - (\zeta u_k^\varepsilon \chi_{u^\varepsilon>0})_t u_t^\varepsilon + \zeta\lambda^\varepsilon \chi_{u^\varepsilon>0} u_k^\varepsilon]\, dz \\
&\xrightarrow[\varepsilon\to 0]{} -\int_{\Omega_T} [\nabla(\zeta v_k)\nabla v - (\zeta v_k \chi_{v>0})_t v_t + \zeta\lambda\chi_{v>0} v_k]\, dz \\
&\qquad (u_k^\varepsilon \to v_k,\ \lambda^\varepsilon \to \lambda \text{ is assumed}) \\
&= \int_{\Omega_T\cap\{v>0\}} \zeta v_k(\Delta v - v_{tt} - \lambda) dz - \int_{\Omega_T\cap\partial\{v>0\}} \zeta v_k\,(\nabla v, -v_t)\cdot \nu dS \\
&= -\int_{\Omega_T\cap\partial\{v>0\}} \zeta v_k(\nabla v, -v_t)\cdot \nu dS \ \ (\Delta v - v_{tt} = \lambda \text{ is assumed}).
\end{aligned}
$$

Note that outer normal to $\{v > 0\}$ is $\nu = -Dv/|Dv|$, where $Dv = (v_{x_1}, \cdots, v_{x_n}, v_t)$. Therefore, we can see that $v_k = -\nu_k|Dv|$ on $\partial\{u > 0\}$. Then, eventually, the left hand side of (2.1) becomes

$$
(\text{l.h.s.}(2.1)) = -\int_{\Omega_T\cap\partial\{v>0\}} \zeta v_k(\nabla v, -v_t)\cdot \nu dS = -\int_{\Omega_T\cap\partial\{v>0\}} \zeta\left[|\nabla v|^2 - (v_t)^2\right]\nu_k dS.
$$

Thus we get the equation

$$
\int_{\Omega_T\cap\partial\{v>0\}} \zeta Q^2 \nu_k dS = \int_{\Omega_T\cap\partial\{v>0\}} \zeta\left[|\nabla v|^2 - (v_t)^2\right]\nu_k dS,
$$

which shows that

$$
|\nabla v|^2 - (v_t)^2 = Q^2 \ \text{ on } \partial\{v > 0\}. \tag{2.2}
$$

The limit boundary condition (2.2) is the same as the one obtained for the hyperbolic free boundary problem introduced in [5]. □

3 Minimizing method for the bubble problem

Like in [8], we introduce another approximation problem to (1.1). Here, we give the volume constraint in the admissible space for finding a minimizer of a discretized functional corresponding to the Lagrangian.

Problem 3.1. *Let Ω be a bounded domain in $\mathbf{R}^m$. For $n = 2, 3, \ldots$, find minimizer u_n of the following functional:*

$$
J_n(u) := \int_\Omega \frac{|u - 2u_{n-1} + u_{n-2}|^2}{2h^2}\chi_{u>0} dx + \frac{1}{2}\int_\Omega |\nabla u|^2 dx + \int_\Omega Q^2 \chi^\varepsilon(u) dx, \tag{3.1}
$$

in the function set

$$
\mathcal{K}_M := \left\{ u \in W^{1,2}(\Omega, \mathbf{R}); u = 0 \ \text{on}\ \partial\Omega,\ \int_\Omega u\, dx = M \right\}.
$$

Functions $u_0, u_1 \in \mathcal{K}_M$ with $u_1 = u_0 + hv_0$ are given and the sequence $\{u_n\}$ is to be determined inductively. Moreover, by use of these minimizers, construct an approximate weak solution to (1.1).

Let us set test function $w^\delta = \frac{u+\delta\zeta}{\int_\Omega (u+\delta\zeta)\,dx}$, $\zeta \in C_0^\infty(\Omega \cap \{u > 0\})$ and take the first variation of J_n:

$$\int_\Omega \left(\frac{u - 2u_{n-1} + u_{n-2}}{h^2} \phi + \nabla u \nabla \phi + Q^2(\chi^\varepsilon)'(u)\phi \right) dx = \int_\Omega \phi \lambda_n dx$$

$$\forall \phi \in C_0^\infty(\Omega \cap \{u > 0\}), \tag{3.2}$$

$$u \equiv 0 \qquad \text{otherwise} \tag{3.3}$$

Here,

$$\lambda_n = \int_\Omega \left(\frac{u - 2u_{m-1} + u_{m-2}}{h^2} u\chi_{u>0} + |\nabla u|^2 \right) dx$$

is the Lagrange multiplier coming from the volume constraint. From the second identity, we can conclude that $u \equiv 0$ outside the set $\{u > 0\}$.

4 Interpolation in time and approximate solution

In this section, we carry out interpolation in time of minimizers $\{u_n\}$ and introduce the approximate weak solution. First we state the definition of *weak solution.*

Definition 4.1. *We call u a weak solution to (1.1), if u satisfies the following:*

$$\int_0^T \int_\Omega \left(-u_t\phi_t + \nabla u \nabla \phi + Q^2(\chi^\varepsilon)'(u)\phi\right) dxdt - \int_\Omega v_0 \phi(x,0)dx = \int_0^T \int_\Omega \lambda \phi dxdt$$

$$\forall \phi \in C_0^\infty(\Omega \times [0,T) \cap \{u > 0\}), \tag{4.1}$$

$$u \equiv 0 \qquad \textit{outside } \{u > 0\} \tag{4.2}$$

and $u(0) = u_0$ in the sense of traces.

Now, we consider the approximate solutions. We define $\bar{u}^h$ and u^h on $\Omega \times (0, \infty)$ by

$$\begin{aligned} \bar{u}^h(x,t) &= u_n(x), \\ u^h(x,t) &= \frac{t - (n-1)h}{h} u_n(x) + \frac{nh - t}{h} u_{n-1}(x), \\ \bar{\lambda}^h(t) &= \lambda_n, \end{aligned}$$

for $(x,t) \in \Omega \times ((n-1)h, nh]$, $n \in \boldsymbol{N}$. We can construct the approximate weak solution to the bubble problem in terms of $\bar{u}^h$ and u^h.

Definition 4.2 (Approximate solution). *Let* $\{u_n\} \subset \mathcal{K}_M$ *and let* $\bar{u}^h$ *and* u^h *be defined as above. If the following conditions*

$$\int_h^T \int_\Omega \left(\frac{u_t^h(t) - u_t^h(t-h)}{h} \phi + \nabla \bar{u}^h \nabla \phi + Q^2 (\chi^\varepsilon(u^h))' \phi \right) dx dt = \int_h^T \int_\Omega \bar{\lambda}^h \phi dx,$$
$$\forall \phi \in C_0^\infty(\Omega \times [0,T) \cap \{u^h > 0\}),$$
$$u^h \equiv 0 \quad \text{in} \quad \Omega \times (h,T) \setminus \{u^h > 0\}$$

and the initial conditions $u^h(0) = u_0$, $u^h(h) = u_0 + hv_0$ *are satisfied, then we call* $\bar{u}^h$ *and* u^h **approximate solutions** *to the bubble problem.*

If one can pass to the limit as $h \to 0$, then the above approximate solutions are expected to converge to the solution of (4.1)-(4.2). We expect that a good regularity of minimizers $\{u_n\}$ should imply that the limit of $\bar{\lambda}^h$ agrees with the Lagrange multiplier λ of (1.3). By now, we could not get any result concerning the convergence of approximate solutions. However, we can still carry out numerical computations using a minimizing method.

5 Numerical method

Here we present the numerical method and experimental results. We apply a finite element method with minimizing algorithm and find minimizer of the approximate functional $J_n(u)$ defined above via steepest descent method for a fixed time step n. The time step h and diameter of each finite element are chosen small enough related to the approximation parameter ε.

In the following simulations, we use equation with a damping term γu_t, i.e.

$$\chi_{u>0} u_{tt} + \gamma u_t = \Delta u - Q^2 (\chi^\varepsilon)'(u) - \lambda \chi_{u>0}.$$

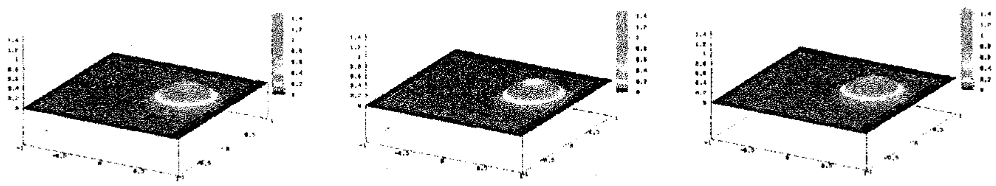
We choose the parameters as follows: $h = 5 \times 10^{-3}$, $\varepsilon = 0.1$, $\gamma = 0.5$.

The first example is calculated under Dirichlet boundary conditions and $Q^2 = 0.35$. An initial velocity is imparted to the bubble. It approaches the boundary of Ω, reflects on the boundary and stops in a certain position.

The second example uses Neumann boundary conditions and $Q^2 = 0.35$. In this case, after touching the boundary, the bubble moves along the boundary. The bubble stops and keeps the smallest surface when reaching the corner of Ω.

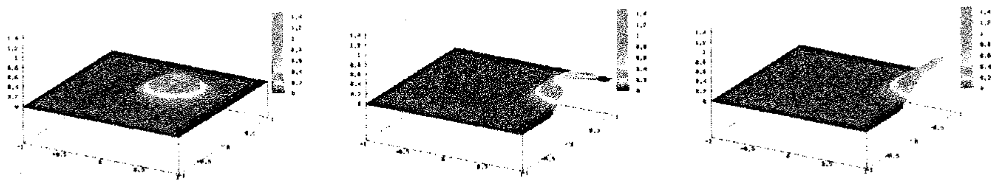
The third example treats a collision of two bubbles with the same volume. After the collision, the bubbles merge.

In the last example we set $Q^2 = 0.03\,(x_1 x_2 > 0)$ and $Q^2 = 0.35$ otherwise. The value of Q^2 determines the contact angle on the free boundary according to the free boundary condition. Therefore, the bubble lies down if Q^2 distribution becomes small and the bubble moves gradually aiming at the part of small Q^2 distribution.



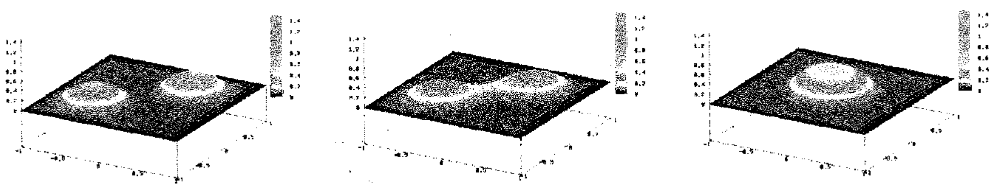
$t = 1.0$ $t = 4.0$ $t = 6.5$

Figure 1: Dirichlet boundary conditions



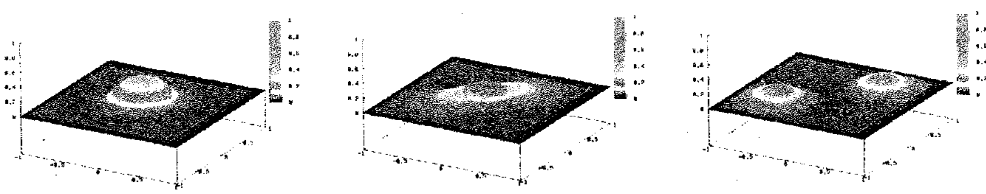
$t = 1.5$ $t = 2.25$ $t = 3.0$

Figure 2: Neumann boundary conditions



$t = 0.0$ $t = 0.80$ $t = 1.500$

Figure 3: Collision of two bubbles with the same volume. $Q^2 = 0.35$.



$t = 0.000$ $t = 0.150$ $t = 1.500$

Figure 4: The bubble is divided to two by the non-uniform distribution of Q^2.

6 Conclusions

A numerical method for a bubble motion with free boundary and volume constraint was developed. The model equation becomes free boundary problem of degenerate hyperbolic type which is difficult to treat. We have introduced a variational method to solve this problem and it gives good numerical results. This model can also be applied to the motion of oil on the bottom of water or to problems related to the phenomenon of a water-drop dripping from ceiling. Therefore, this work has many applications and is significant for the future studying of hyperbolic free boundary problems. It is reported about the former example that the gradient of temperature, wetness or areal density of surface activator makes oil droplet run on the bottom plane and the droplet repeats the division and union while moving (see [10]). And we are now involved in the development of numerical algorithm which describes the division and union of multiple bubbles.

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