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水面に拘束されたバブルの運動の数値シミュレーション
Numerical simulation of motion of a bubble restrained to water surface

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Abstract. The aim of this paper is to develop the numerical method for solving the hyperbolic free-boundary problem under the volume conservation constraint. The equation treated in this paper has a degenerate hyperbolic operator and non-local term (Lagrange multiplier) coming from volume constraint. The typical phenomena described by this equation are the motion of bubble on water surface and oil droplet motion on a plane. We try to realize them numerically. It is the method called *discrete Morse flow (DMF) of hyperbolic type* that plays an important role in the numerical simulation or the stage of construction of an approximate weak solution. The DMF is based on the variational method using time-semidiscretized functional and is suitable to treat a volume constraint condition.

1 Introduction

In this paper, we treat numerically the motion of a bubble which moves on a water surface or an oil droplet on a flat plane. There are some common features in these phenomena. The first common feature is that the volume does not change along their motion. The second common feature of these phenomena is that the area where the bubble or oil droplet exist is localized. We call the set of points where the bubble touches the water surface or where the surface of oil droplet touches the plane *free-boundary.* In this section we explain the model equation that rules the motion of the bubble. However, the model of the bubble can be applied also to the motion of the oil droplet because of these two common properties.

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, areal density of film is expected to be constant, and the stress tensor density of the bubble and water surface to be homogeneous and isotropic.

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

$$\chi_{u>0}\, u_{tt} = \Delta u - R^2 \chi'_\varepsilon(u) + \lambda \chi_{u>0} \quad (x \in \Omega,\, 0 < t < \tau). \tag{1.1}$$

Here Ω is a bounded domain in $\mathbf{R}^m$ (in the following, to simplify the notation, $\Omega_\tau = \Omega \times (0,\tau) \subset \mathbf{R}^{m+1}$ is used), and $\chi_{u>0}$ is the characteristic function of the set $\{u > 0\}$ and $\chi_\varepsilon \in C^2(\mathbf{R})$ is a smoothing of χ satisfying

$$\chi_\varepsilon(s) = \begin{cases} 0, & s \le 0 \\ 1, & \varepsilon \le s \end{cases}$$

with interpolating in $0 < s < \varepsilon$ in such a way that $|\chi'_\varepsilon(s)| \le C/\varepsilon$. The term $R^2\chi'_\varepsilon(u)$ describes the net adhesive force. It is due to this restriction force that the generation of the new surface or movement of free-boundary are obstructed. The specificity of equation (1.1) lies in the coefficient $\chi_{u>0}$ on the left-hand side. Because of this coefficient, non-negativity of the solution is guaranteed. Function λ, which appears in the last term of (1.1) is a Lagrange multiplier originating in the volume preservation condition. The explicit form of the Lagrange multiplier λ is obtained as follows:

$$\lambda = \frac{1}{M}\int_\Omega \left[u u_{tt}\, \chi_{u>0} + |\nabla u|^2 + R^2 u \chi'_\varepsilon(u)\right] dx \tag{1.2}$$

by formal calculation with volume constraint under the assumption that λ does not depend on space variables. 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]).

2 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 2.1. *Let Ω be a bounded domain in $\mathbf{R}^m$. For $n = 2, 3, \ldots$, find minimizer u_n of the following functional:*

$$J_n(u) := \int_\Omega \frac{|u - 2u_{n-1} + u_{n-2}|^2}{2h^2}\,dx + \frac{1}{2}\int_\Omega |\nabla u|^2\,dx + \int_\Omega R^2 \chi_\varepsilon(u)\,dx, \tag{2.1}$$

in the function set

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

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 use test function $(u+\delta\zeta)/\int_\Omega (u+\delta\zeta)\chi_{u+\delta\zeta>0}\,dx$, $\zeta \in C_0^\infty(\Omega\cap\{u>0\})$ and take the first variation of J_n:

$$\int_\Omega \left(\frac{u-2u_{n-1}+u_{n-2}}{h^2}\zeta + \nabla u\nabla\zeta + R^2\chi_\varepsilon'(u)\zeta\right)dx = \int_\Omega \zeta\lambda_n dx$$
$$\forall\zeta \in C_0^\infty(\Omega\cap\{u>0\}), \tag{2.2}$$
$$\int_\Omega \nabla u\nabla\zeta\,dx = 0 \qquad \forall\zeta \in C_0^\infty(\Omega\cap\{u\le 0\}^\circ). \tag{2.3}$$

Here,
$$\lambda_n = \int_\Omega \left(\frac{u-2u_{m-1}+u_{m-2}}{h^2}u + |\nabla u|^2 + R^2\chi_\varepsilon'(u)\,u\right)dx$$
is the Lagrange multiplier coming from the volume constraint. From the second identity, we can conclude that $u\equiv 0$ outside the set $\{u>0\}$.

3 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 3.1. *We call u a weak solution to (1.1), if u satisfies the following:*

$$\int_0^T\int_\Omega \left(-u_t\zeta_t + \nabla u\nabla\zeta + R^2\chi_\varepsilon'(u)\zeta\right)dxdt - \int_\Omega v_0\zeta(x,0)dx = \int_0^T\int_\Omega \lambda\zeta dxdt$$
$$\forall\zeta \in C_0^\infty(\Omega\times[0,T)\cap\{u>0\}), \tag{3.1}$$
$$u\equiv 0 \qquad \text{outside of } \{u>0\} \tag{3.2}$$

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 3.2 (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*

$$\int_h^T \int_\Omega \left(\frac{u_t^h(t) - u_t^h(t-h)}{h} \zeta + \nabla \bar{u}^h \nabla \zeta + R^2 \chi_\varepsilon' \left(u^h\right) \zeta \right) dx dt = \int_h^T \int_\Omega \bar{\lambda}^h \zeta \, dx,$$

$$\forall \zeta \in C_0^\infty \left(\Omega \times [0, T) \cap \left\{u^h > 0\right\} \right),$$

$$u^h \equiv 0 \qquad \text{in } \Omega \times (h, T) \setminus \left\{u^h > 0\right\}$$

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 (3.1)-(3.2). 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 (1.1). 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.

4 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. However, the functional (2.1) does not correspond to the case when two or more bubbles exist. In that case, we should detect each bubble and find minimizer for each bubble. After detection of each bubble, the basic course of our minimizing algorithm is the following:

1. $u_0, u_1 (= u_0 + hv_0) \in \mathcal{K}_M$ is an initial value

2. for $n = 1, 2, \ldots, N$, determine u_{n+1} by the following procedure

- **a.** $v^1 = u_n$
- **b.** for $k = 1, 2, \ldots, K_n$
  (K_n is made so large that a certain error estimator becomes small enough)
  - **i.** $p^k = \nabla_u J_n \left(v^k\right)$ as retrieval direction
  - **ii.** search the minimizer $\widetilde{v}^{k+1}$ in the direction $-p^k$
    (steepest descent method + bisection method)
  - **iii.** $\hat{v}^{k+1} = \max\left\{\widetilde{v}^{k+1}, 0\right\}$
  - **iv.** projection onto the volume-constraint plane:
    $v^{k+1} = \mathcal{P}\left(\hat{v}^{k+1}\right)$
- **c.** $u_{n+1} = v^{K_n+1}$

By executing tasks **a.** – **c.**, we get an approximate minimizer for a fixed time step n.

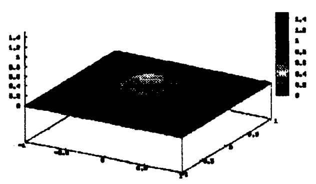
In the following simulations, we use equation with a damping term γu_t, i.e.

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

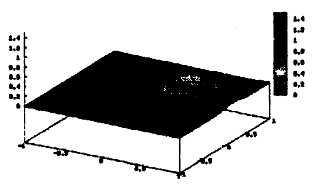
We choose the parameters as follows: $h = 5 \times 10^{-3}$, $\varepsilon = 0.1$, $\gamma = 0.5$.

4.1 Neumann condition

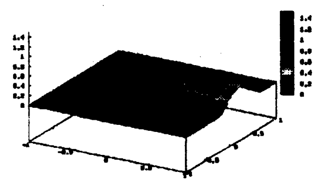
The first example uses Neumann boundary condition and $R^2 = 0.35$. An initial velocity is imparted to the bubble. In this case, it approaches the boundary of Ω. After touching the boundary, the bubble moves along the boundary. The more the bubble leans against the boundary, the smaller the area of the surface of the bubble becomes. The bubble stops and keeps the smallest surface when reaching the corner of Ω.



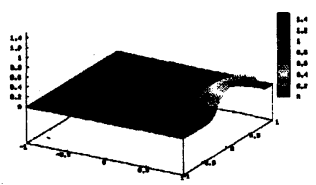
(a) $t = 0.0$



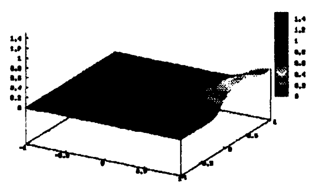
(b) $t = 1.75$



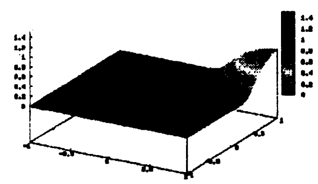
(c) $t = 2.2$



(d) $t = 2.65$



(e) $t = 6.35$

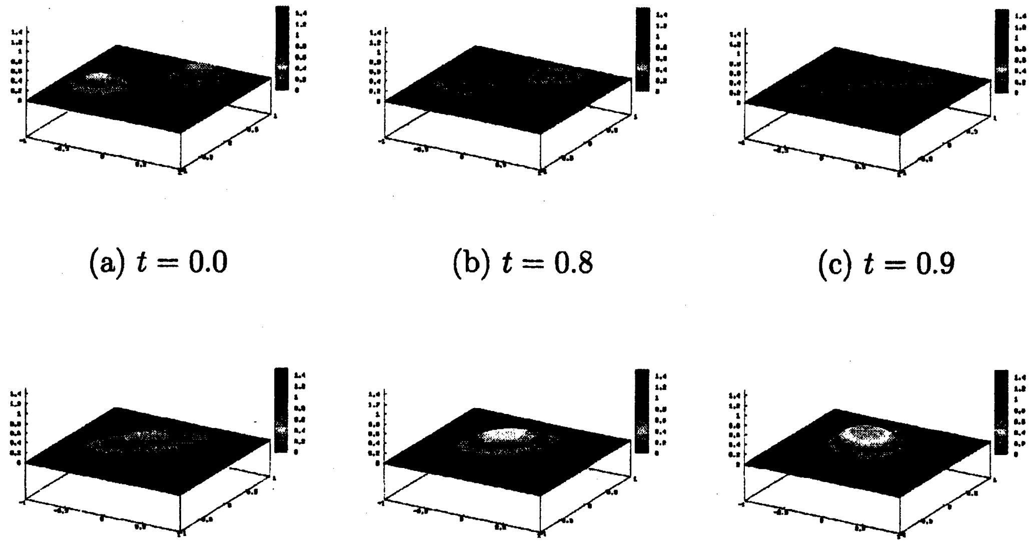


(f) $t = 8.0$

Figure 1: Neumann boundary condition. The bubble which has an initial velocity chosen in such away that it moves diagonally, moves toward the boundary. After touching the boundary, the bubble moves along it and finds the corner of the domain.

4.2 Collision of two bubbles

The second example treats a collision of two bubbles with the same volume. After the collision, the bubbles merge and keep the smallest surface near the center of initial position of two bubbles.



(a) $t = 0.0$ (b) $t = 0.8$ (c) $t = 0.9$

(d) $t = 1.1$ (e) $t = 1.2$ (f) $t = 1.5$

Figure 2: collision of two bubbles. Two bubbles separated initially merge into each other.

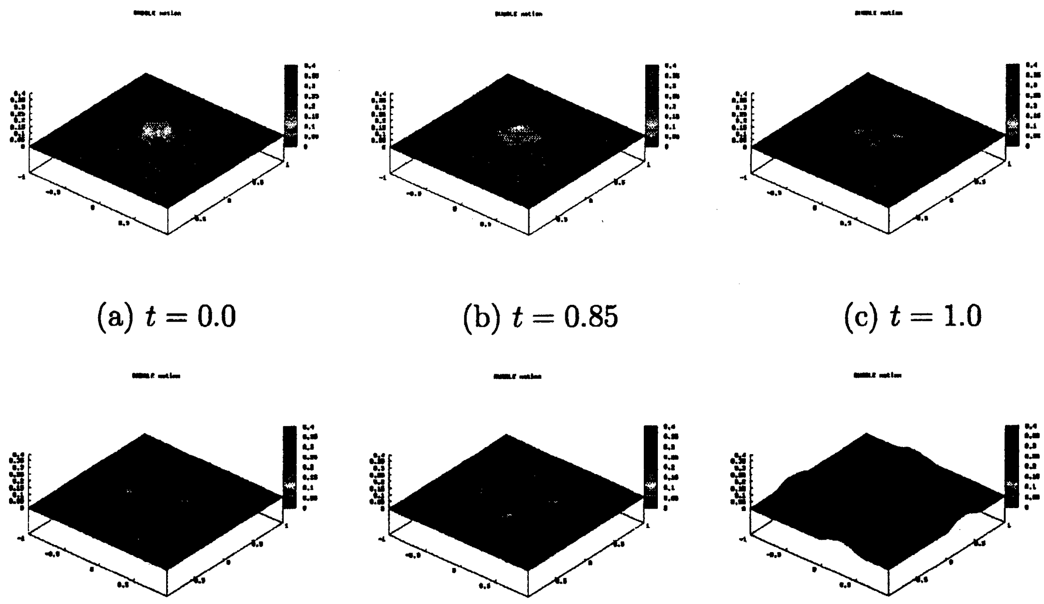
4.3 Division of oil droplet

In the third example, the motion of oil drople on the flat plane on which there is a nonuniform distribution of surface-active agent is considered.

The contact angle between the oil droplet and the plane is prescribed by the affinity of the material of the water surface to the oil droplet surface. Therefore, if there is a nonuniform distribution of surface-active agent, we can observe that the oil droplet moves on the plane driven by the force of non-uniformity of the contact angle. The free-boundary condition

$$|\nabla u|^2 - (u_t)^2 = R^2 \quad \text{on } \partial\{v > 0\}, \tag{4.1}$$

which is obtained by passing to the limit as $\varepsilon \to 0$ in (1.1) tells us that we can rule the contact angle of the oil droplet and the plane by defining the coefficient R. The oil droplet lies down if R^2 distribution becomes small and the droplet moves gradually



(a) $t = 0.0$ (b) $t = 0.85$ (c) $t = 1.0$

(d) $t = 1.15$ (e) $t = 1.2$ (f) $t = 1.5$

Figure 3: Division of bubblc (case 2).

aiming at the part of Ω with smaller R^2. We set

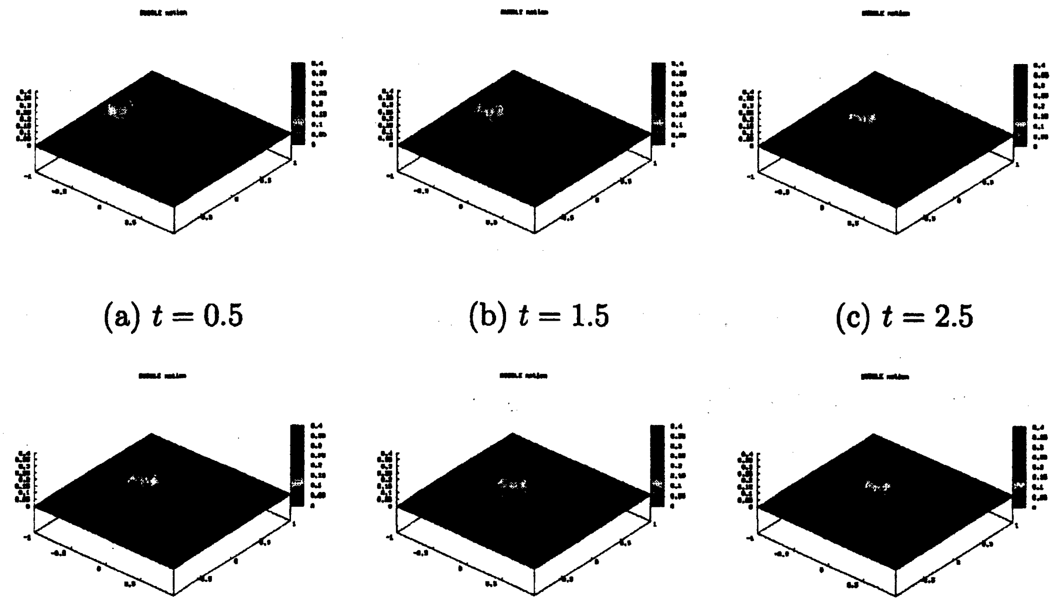
$$R^2 = \begin{cases} 0.35 & (x_1 x_2 (x_1^2 - x_2^2) \leq 0) \\ 3.5 & \text{otherwise.} \end{cases}$$

4.4 Combination with reaction-diffusion equation

In [11] it is reported that an oil droplet on the glass plane immersed in surface-active agent solution immediately moves according to the gradient of the concentration of the surface-active agent. We are trying to realize the motion of the oil droplet numerically by applying the model of the bubble (1.1) to this phenomenon and combining it with reaction-diffusion equation which shows the time development of the concentration of surface-active agent. Let v be the concentration of surface-active agent, then our model equation of v is as follows:

$$\begin{aligned} R^2 &= \left(\frac{Q}{T}\right)^2 + \frac{\gamma_w(v) - \gamma_b}{T}, \\ v_t &= \kappa \Delta v + \mu (v_0 - v) v \chi_{u \leq 0} - \nu v \chi_{u > 0}, \\ \gamma_w &= \frac{\gamma_0}{1 + \alpha v^\beta}. \end{aligned}$$

Here T is the tension of the oil droplet surface, γ_w is the tension of glass plane surface and γ_b expresses the tension of the region where both the oil droplet and glass plane surface have come in contact, $Q > 0$ is adhesion between the oil and the surface of plane. In the numerical experiment we set $\alpha = 1$, $\beta = 2$ and impose Neumann boundary condition. We choose the uniform distribution as the initial condition for v. We use the explicit method to solve this equation. It is observed that the oil droplet put near the boundary starts moving aiming at the area where the concentration of the surface-active agent is high. However, the droplet slows down and stops before reaching the center of the domain, although it should keep moving as the experiment shows. We think that it is necessary to improve the model, e.g. by considering the internal energy of the oil in addition to the surface energy.



(a) $t = 0.5$ (b) $t = 1.5$ (c) $t = 2.5$

(d) $t = 3.0$ (e) $t = 4.0$ (f) $t = 4.5$

Figure 4: Combination with the reaction-diffusion system.

5 Conclusions

We model the motion of a bubble on a water surface by a free-boundary problem with volume conservation constraint and we have established a numerical method for its solution. The bubble moves on the water surface while changing its shape but preserving its volume. The model equation becomes free-boundary problem of degenerate hyperbolic type which is difficult to treat. We have introduced the time-semidiscretized 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.

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