Simulation of The Motion of A Droplet on A Plane by The Discrete Morse Flow Method

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Abstract. *This research concerns the simulation of the motion of a droplet on a plane. We study the film which represents the surface of the droplet [5]. The evolution of the film is described by the hyperbolic equation with the volume preservation, which means that the volume between the film and the surface where the droplet rests does not change in time. Moreover free boundary appears as a moving boundary of the drop. The hyperbolic free boundary problem under the volume preservation condition is solved by the discrete Morse flow method (DMF).*

Keywords: droplet, volume preservation, free boundary, discrete Morse flow method

1 Introduction

The model of the motion of a droplet on a plane consists of two related parts: the film of the droplet and fluid inside the film. In this work, we only study the film which represents the surface of the droplet. The crucial features of the drop are the volume preservation, free boundary and positive contact angle.

The shape of the surface of the drop can be represented by the graph of a scalar function

$$u : \Omega \times (0,T) \to (0,\infty),$$

where Ω is a domain in $\mathbb{R}^2, T$ is the positive real number and $(0,T)$ is the time interval.

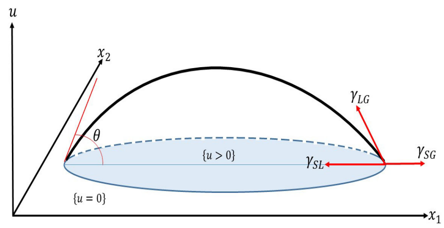

Figure 1: Droplet on a plane.

The contact angle is assumed to be small and depend on the surface tensions described by Young's equation

$$\gamma_{SG} - \gamma_{SL} = \gamma_{LG} \cos\theta.$$

where γ_{SG} is the solid surface tension,γ_{LG} is the liquid surface tension,γ_{SL} is the solid/liquid interfacial surface tension.

Furthermore, the volume preservation of the film is assumtion

$$\int_\Omega u dx = V,$$

where V is the positive constant.

This problem is solved by the discrete Morse flow method.

2 Derivation of the film equation

In this section, we derive the film equation by calculating the first variation of the action function of this phenomena. In order to define the action function, we have to consider the kinetic energy and the potential energy of this problem. For the portential energy, we consider the surface energy of the droplet which can be written as

$$E = \int_\Omega \gamma_g \sqrt{1+|\nabla u|^2}\chi_{u>0} dx + \int_\Omega \gamma_s \chi_{u>0} dx, \tag{1}$$

where $\gamma_g = \gamma_{LG}, \gamma_s = \gamma_{SL} - \gamma_{SG}, \chi_{u>0}$ the characteristic function.

By the assumtion of θ, $|\nabla u|$ remains small. So the following Taylor approximation is available

$$\sqrt{1+|\nabla u|^2} \approx 1 + \frac{1}{2}|\nabla u|^2. \tag{2}$$

Then by the approximation 2, the equation 1 can be approximated as

$$\tilde{E} = \int_\Omega \frac{\gamma_g}{2}|\nabla u|^2 dx + \int_\Omega R^2 \chi_{u>0} dx, \tag{3}$$

where $R^2 = \gamma_s + \gamma_g$.

The kenetic energy of the film given by

$$\int_\Omega \frac{\sigma}{2} u_t^2 \chi_{u>0} dx, \tag{4}$$

where σ is the area density of the surface.

Hence, the Lagrangian of this problem can be expressed as

$$L(u) = \int_\Omega (\frac{\sigma}{2} u_t^2 \chi_{u>0} - \frac{\gamma_g}{2}|\nabla u|^2 - R^2 \chi_\epsilon(u)) dx, \tag{5}$$

where χ_ϵ is the smoothing function of the characteristic function given by

$$\chi_\epsilon(u) = \begin{cases} 1, & u \geq \epsilon, \\ 0, & u \leq 0. \end{cases}$$

and $|\chi'(u)| \leq C/\epsilon$ for $u \in (0, \epsilon)$. In order to avoid the existence of the delta function, we use χ_ϵ instead of $\chi_{u>0}$ [7].

The action function within time interval $(0, T)$ can be written as

$$J(u) = \int_0^T L(u) dt \tag{6}$$

We have to seek a stationary point of the action function 6 in the following set

$$K = \{u \in H^1(\Omega \times (0,T)); u|_{\partial\Omega} = 0, \int_\Omega u\chi_{u>0} dx = V\}.$$

By assuming the existence of a stationary point, the first variation of the action function is

$$\frac{d}{d\epsilon} J(u_\epsilon)|_{\epsilon=0} = 0,$$

with using the following test function and its volume are

$$\varphi \in C_0^\infty((0,T) \times \Omega \cap \{u > 0\}), \qquad \Phi = \int_\Omega \varphi(t,x)dx.$$

and denoting

$$u_\epsilon = V \frac{u + \epsilon\varphi}{V + \epsilon\Phi}.$$

We arrive at the following equation

$$\begin{aligned} 0 &= \int_0^T \int_\Omega (\chi_{u>0}\sigma u_t \varphi_t - \gamma_g \nabla u \nabla \varphi - R^2 \chi'_\epsilon(u)\varphi) dxdt \qquad (7) \\ &+ \frac{1}{V} \int_0^T \int_\Omega (-\sigma u_t (u\Phi)_t \chi_{u>0} + \gamma_g |\nabla u|^2 \Phi + R^2 u \chi'_\epsilon(u)\Phi) dxdt. \end{aligned}$$

Let us consider the last term on the right hand side of the equation 7, we integrate this by parts respect to time, we attain to

$$\begin{aligned} &\frac{1}{V} \int_0^T \int_\Omega (-\sigma u_t (u\Phi)_t \chi_{u>0} + \gamma_g |\nabla u|^2 \Phi + R^2 u \chi'_\epsilon(u)\Phi) dxdt \\ &\quad = \frac{1}{V} \int_0^T \int_\Omega (\sigma u u_{tt} \chi_{u>0} + \gamma_g |\nabla u|^2 + R^2 u \chi'_\epsilon(u))\Phi dxdt \end{aligned}$$

By denoting the Lagrange multiplier of this problem as

$$\lambda = \frac{1}{V} \int_\Omega (\sigma u u_{tt} \chi_{u>0} + \gamma_g |\nabla u|^2 + R^2 u \chi'_\epsilon(u)) dx.$$

We get the following relation

$$\int_0^T \int_\Omega (-\chi_{u>0}\sigma u_t \varphi_t + \gamma_g \nabla u \nabla \varphi + R^2 \chi'_\epsilon(u)\varphi - \lambda\varphi) dxdt = 0. \qquad (8)$$

The governing equation of the film is the strong from of above relation which can be expressed as

$$\chi_{u>0}\sigma u_{tt} = \gamma_g \Delta u - R^2 \chi'_\epsilon(u) + \lambda, \qquad (9)$$

For our problem, we consider the film equation with damping term, $\mu u_t(t,x)$, which is the resistance force acting against the vertical motion of the film. It can be represented by the speed of the film with constant μ in [5]. By defining $\gamma = 1 + \frac{\gamma_s}{\gamma_g}$ and choosing $\sigma = 1, \gamma_g = 1$. We only consider the positive solution of the following equation with the initial and boundary conditions

$$\begin{cases} \chi_{u>0} u_{tt}(t,x) = -\mu u_t(t,x) + \Delta u(t,x) - \gamma \chi_\epsilon'(u) + \chi_{u>0}\lambda(t) \quad \text{in} \quad (0,T)\times\Omega, \\ u(t,x) = 0 \quad \text{on} \quad (0,T)\times\partial\Omega, \\ u(0,x) = u_0(x) \quad \text{in} \quad \Omega, \\ u_t(0,x) = v_0(x) \quad \text{in} \quad \Omega, \end{cases} \tag{10}$$

where $u_0(x)$ and $v_0(x)$ are the initial shape and the initial velocity, respectively, and the Lagrange multiplier is

$$\lambda = \frac{1}{V}\int_\Omega (uu_{tt} + \mu u_t u + |\nabla u|^2 + \gamma u \chi_\epsilon'(u))dx.$$

3 Discrete Morse flow method

The discrete Morse flow is the variational method used to solved the problem that dependent on time. The method was first presented to solve parabolic problem by N.Kikuchi in [6] and further applied to hyperbolic problem later in [2] and others. Moreover, it was also applied to solve the numerical solution of the free boundary problem in [1],[3] and the volume-preserving problem in [4],[5].

We fix a non negative integer $N > 0$, set the time step $h = T/N$. We seek a sequence $\{u_n\}$ by minimize the following functional for our problem see [5]

$$J_n(u) = \int_\Omega \left(\frac{|u - 2u_{n-1} + u_{n-2}|^2}{2h^2}\chi_{u>0} + \mu\frac{|u-u_{n-1}|^2}{2h} + \frac{|\nabla u|^2}{2} + \gamma\chi_\epsilon(u)\right)dx, \tag{11}$$

on the set

$$K_v = \{u \in H_0^1; \int_\Omega u\chi_{u>0}dx = V\}.$$

where the sequence $\{u_n\}$ determine by u_0 is the initial shape, $u_1 = u_0 + hv_0$ and for $n = 2, 3, 4, ...$ u_n are the minimizer of the functional 11 on the set K_v.

4 Algorithm

We can find the sequence of minimizer, $\{u_n\}$, of our functional 11 by the following algorithm

1. Given the initial shape, u_0 and initial velocity, v_0, put $u_1 = u_0 + hv_0$.
2. For $n = 1, 2, \cdots, N$, we can seek u_{n+1} as follows:
   (a) $p^1 = u_n, k = 1$.
   (b) Repeat the following.
      - search for the minimizer $\tilde{p}^{k+1}$ of J_n,
      - $p^{k+1} = \max(\tilde{p}^{k+1}, 0)$,
      - project p^{k+1} on the volume constraint hyperplane $v^{k+1} := \text{Proj}(\tilde{v}^{k+1})$,
      - if the convergence criterion is fulfilled, leave the loop, else $k = k + 1$.

   (c) $u_{n+1} = p^{k+1}$.

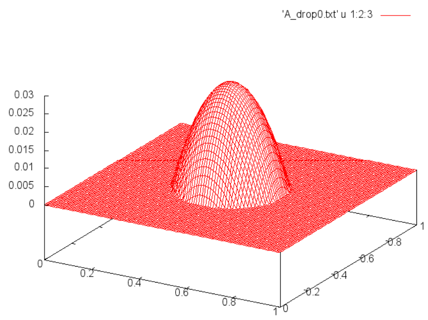

Figure 2: $t = 0$

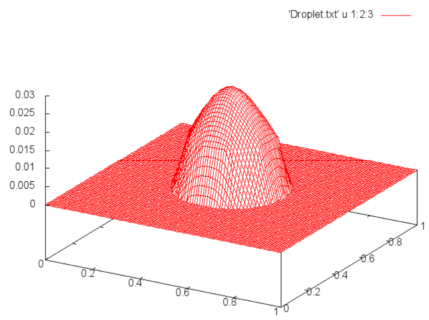

Figure 3: $t = 1$

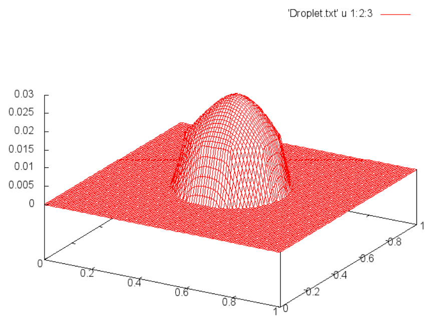

Figure 4: $t = 4$

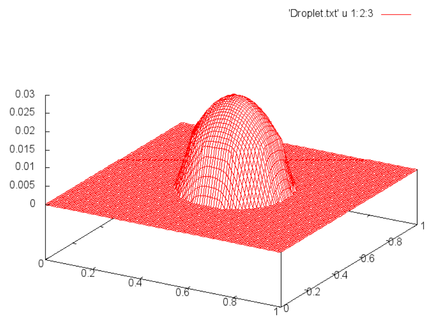

Figure 5: $t = 20$

5 Numerical approach

In this section, we use the spherical cap represented the shape of the drop for the initial shape and given the velocity of the drop into the suitable direction. By using the discrete Morse method for our problem where the radius of the drop is 0.85, the contact angle is $15°$, ϵ is 0.01294 and the time step is 7.5×10^{-3} . The results is presented on above.

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