Simulation of Triple Line Dynamics by Interface-Fluid Coupling

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Nur Shofianah
Graduate School of Natural Science and Technology, Kanazawa University

Abstract

The thesis develops a coupled interface-network and fluid model which can serve as a first step to simulate triple line dynamics. The main ingredients of this coupled model are the interface model with nonsymmetric junctions and the fluid model in moving domain. We build an interface model based on the gradient flow of surface energy and develop a method for its numerical solution by generalizing the reference vectors and diffusion system in vector-valued BMO algorithm. Moreover, we improve the scheme by using vector-valued projection triangle and use a vector type DMF to handle volume constraint via penalization. For the fluid part, we implement a numerical method adopting DSD/SST-SUPS, a stabilized space-time finite element method in moving domain. We also apply the appropriate boundary condition which is related with a moving triple line. We couple these two models weakly via pressure acting from the fluids on the interfaces and by the fact that the interfaces determine the domain for fluid motion. In the end, we present results of numerical experiments.

We develop a coupled interface-network and fluid model which can serve as a first step to simulate triple line dynamics. We derive equation of triple junction and adopt Navier-Stokes equation for incompressible flow as the basic of interface model and fluid model, respectively. For each model, we develop a method for its numerical solution.

We take rising bubble at the bottom of the container filled with fluid as an example of the problem. The physical setting of the problem is depicted in the Fig.1. We solve incompressible Navier-Stokes equation in P_2 and consider the motion of the interface according to mean curvature. Here, the moving triple lines are free boundary so we need one more boundary condition by deriving the equation of triple junction to know how the triple junction evolves under gradient flow of surface energy. We consider three evolving curves $\gamma_i(s)$, $s \in [p_i, q_i], i = 1, 2, 3$, which lie inside a fixed smooth region Ω of $\mathbb{R}^2$, meet the outer boundary $\partial\Omega$ at a right angle and get together at a triple junction $x_T = \gamma_i(q_i)$. Each curve has different surface tension σ_i. The motion by gradient flow satisfies

1. The normal velocity of interface: $v_i = \sigma_i \kappa_i$.
2. The Force balance condition at triple junction: $\sum_{i=1}^{3} \sigma_i \boldsymbol{t}_i = 0$.

The coupling problem can be formulated as follows,

$$
\begin{aligned}
v_3 &= \sigma_3\, \kappa_3 + p, \ \text{ at } \ \gamma_3(t), \\
\sum_{i=1}^{3} \sigma_i t_i &= 0, \ \text{ at } \ (x_{TL})(t), \\
\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} - \mathbf{f}\right) - \nabla\cdot(-p\mathbf{I} + 2\mu\boldsymbol{\varepsilon}(\mathbf{u})) &= \mathbf{0}, \ \text{ in } \bigcup_{t\in(0,T)} P_2(t)\times\{t\}, \\
\nabla\cdot\mathbf{u} &= \mathbf{0}, \ \text{ in } \bigcup_{t\in(0,T)} P_2(t)\times\{t\}.
\end{aligned}
$$

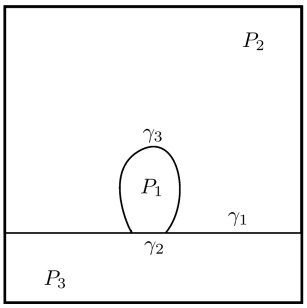

Fig.1 Rising bubble at the bottom of the container filled with fluid

In order to realize nonsymmetric junction motion with stable junction angles and correct interface velocity, we generalize the reference vectors and diffusion system in vector-valued BMO algorithm. First, we investigate the condition on the selection of general reference vectors, i.e.,

$$\theta_1\mathbf{p}_1 + \theta_2\mathbf{p}_2 + \theta_3\mathbf{p}_3 = \mathbf{0}. \tag{1}$$

Since the reference vectors are determined up to rotation and scaling, we can choose one reference vector arbitrarily, e.g., $\mathbf{p}_3 = (1, 0)$ and find the remaining,

$$
\begin{aligned}
\mathbf{p}_1 &= \left(1 - \frac{2\pi}{\theta_1\theta_3}(\pi - \theta_2),\ \pm\frac{2}{\theta_1\theta_3}\sqrt{\pi(\pi-\theta_1)(\pi-\theta_2)(\pi-\theta_3)}\right), \\
\mathbf{p}_2 &= \left(1 - \frac{2\pi}{\theta_2\theta_3}(\pi - \theta_1),\ \mp\frac{2}{\theta_2\theta_3}\sqrt{\pi(\pi-\theta_1)(\pi-\theta_2)(\pi-\theta_3)}\right).
\end{aligned}
$$

Second, we consider general diffusion system,

$$\begin{cases} u_t^1 + du_t^2 = a\Delta u^1 + b\Delta u^2, \\ du_t^1 + eu_t^2 = b\Delta u^1 + c\Delta u^2, \\ \begin{pmatrix} u^1 \\ u^2 \end{pmatrix}(t=0) = \begin{pmatrix} u_0^1 \\ u_0^2 \end{pmatrix}, \end{cases}$$

and determine its coefficients a, b, c, d, e, so that we obtain the desired interface velocities. By transforming the system, applying some computations, and setting $d = 0,\ e = 1$, we get appropriate general diffusion system

$$\mathbf{u}_t = A\Delta\mathbf{u}, \qquad A = \begin{pmatrix} a & b \\ b & c \end{pmatrix},$$

with interface velocity

$$v_k = \frac{\mu_1(a+c+r) + 2\mu_2\sqrt{ac-b^2}}{\mu_2(a+c+r) + 2\mu_1\sqrt{ac-b^2}}\sqrt{ac-b^2}\,\kappa_k,$$

leading a nonlinear system consisting of three equations for the coefficients a, b and c, which is solved numerically. Here, μ_1, μ_2 depend on a, b, c and reference vectors, and $r = \sqrt{(a-c)^2 + 4b^2}$.
We have observed that no matter how we change the diffusion system, the stability condition (**??**) will not be affected.

At this stage, for the case with initial configuration of three straight lines meeting at the junction with stable contact angles, we have shown that for a suitably selected reference vectors, the junction will be stationary, and that, for a suitably selected diffusion system, if an interface point is sufficiently far from the junction, the interface velocity at that point will satisfy the desired formula $v_i = \sigma_i\kappa_i$. However, the above analysis does not address the close vicinity of the triple junction. By formal calculations it can be made clear that the correct interface velocity is obtained only with an exponentially decreasing error with respect to the distance of the considered interface point to the junction. This fact is also confirmed by numerical tests. Therefore, we include a correction step based on the notion of a projection triangle given by Ruuth (1998). The idea is to first investigate how the stable configuration of three straight lines deforms, and use this information to project the phase regions back into the correct position in each step of the BMO algorithm. We extended the original projection triangle method in vector-valued formulation.

Using all the analysis above, we develop generalized vector-valued BMO algorithm to realize nonsymmetric junction motion: for given surface tensions σ_i, calculate junction angles θ_i, define general reference vectors $\mathbf{p}_i$, find the coefficients a, b, c of general diffusion system, construct projection triangle, repeat until desired time solving general diffusion system and tresholding according to projection triangle. We solve general diffusion system by using vector-type discrete Morse flow (DMF), i.e., at each step we solve it by discretizing time $\Delta t = h \times N$ and successively minimizing the following functionals for $n = 1, .., N$ over $H^1(\Omega; R^2)$:

$$J_n(\mathbf{u}) = \int_\Omega \left(\frac{a}{2}|\nabla u^1|^2 + b\nabla u^1 \cdot \nabla u^2 + \frac{c}{2}|\nabla u^2|^2\right) \mathrm{d}x + \int_\Omega \left(\frac{|\mathbf{u} - \mathbf{u}_{n-1}|^2}{2h}\right) \mathrm{d}x.$$

We approximate the functional by using piecewise linear finite elements. The minimizers are found by steepest descent method. The minimization formulation of the vector-valued algorithm allows the inclusion of volume constraints via penalization. Here, we minimize

$$F_n(\mathbf{u}) = J_n(\mathbf{u}) + \frac{1}{\epsilon}\sum_{i=1}^{3} |V_i - meas(P_i^{\mathbf{u}})|^2,$$

where $\epsilon > 0$ is a small penalty parameter, V_i is the prescribed volume of region P_i and the volumes corresponding to $\mathbf{u}$ are obtained from the sets

$$P_i^{\mathbf{u}} = \{x \in \Omega; \mathbf{u}(x) \in R_i\},$$

where R_i are the regions of projection triangle. Note that the volume preservation is important for stable weak coupling.

We show some numerical examples. Figure 2.a shows the evolution of triple junction $150°-90°-120°$ with initial T-junction. Notice that for the first 10 time steps, the junction angles rapidly adjusts to approximate $150°-90°-120°$. Thereafter, the triple junction maintains phase interior angles of measure within 2.5% relative error (Figure 2.b)

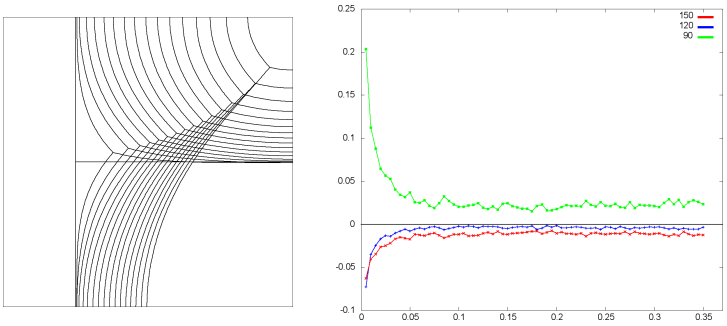

Fig.2(a) Evolution of triple junction motion $150°-90°-120°$ (b) Relative error of junction angles at each time step

Figure 3.a shows the evolution of triple junction with $135°-90°-135°$ with initial T-junction. Note that since the surface tensions on the $1-2$ and $2-3$ interfaces are equal, that is, $\sigma_1 = \sigma_3 = \frac{1}{\sqrt{2}}$, we expect these interfaces to symmetrically evolve with respect to the horizontal line $y = 0.5$. This is in agreement with our numerical simulation shown in Figure 3.a. Moreover, we note that the shape of such a constantly transported profile in the axially symmetric case is determined by: $v(y) = -\frac{2}{\pi}\log(\cos(\frac{\pi}{2}y)) + c$, where the constant c of horizontal shift may be chosen appropriately. Comparing this with the numerical interface solution obtained via our method, we see that it is in a good agreement with the exact shape of the profile (Fig.3.b).

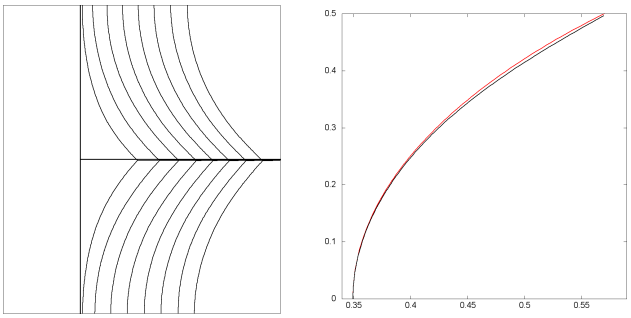

Fig.3(a) Evolution of triple junction motion $135°-90°-135°$ (b) The shape of the numerical interface at time $t = 30\Delta t$ (black) vs the constantly transported solution (red)

Fig. 4 shows a result of volume preserving double bubble simulation. We have observed that the stationary numerical solution well preserves the initial phase volumes.

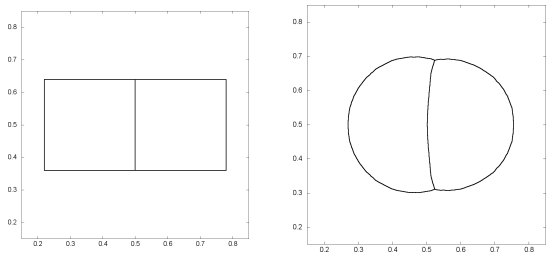

Fig.4(a) Initial condition (b) the stationary numerical solution in case $(150°-90°-120°)$

On the other hand, we build numerical method of fluid model by adopting a stabilized space-time finite element method in moving domain, Deforming-Spatial Domain/Stabilized Space-Time SUPG-PSPG (DSD/SST-SUPS), based on Streamline-Upwind/Petrov-Galerkin (SUPG) stabilization and Pressure-Stabilizing/Petrov-Galerkin (PSPG) stablization. These stabilization terms assure the numerical stability of the computations in advection-dominated flows and when using equal order interpolation functions for velocity and pressure which simplifies implementation. In space-time finite element method, the discretization is applied not only in space but also in time. The formulation of DSD/SST is written over a sequence of spacetime slab Q_n, where Q_n is the slice of the space-time domain between the time levels t_n and t_{n+1}. DSD/SST-SUPS formulation consists of Galerkin formulation of the problem with additional terms, jump term and stabilization terms. The jump term enforces weakly the temporal continuity of the velocity field since the basis functions are discontinous from one space-time slab to another.

After space-time discretization, we obtain a nonlinear system of equations

$$\mathbf{K}(\mathbf{U})\mathbf{U} = \mathbf{F}$$

For each time step. we linearize it using Newton-Raphson method. We compute a correction $\Delta\mathbf{U}$ of a current solution $\mathbf{U}^l$ at each iteration l, which yields a linear system

$$\mathbf{J}(\mathbf{U}^l)\,\Delta\mathbf{U}^l = \mathbf{F} - \mathbf{K}(\mathbf{U}^l)\mathbf{U}^l,$$

where $\mathbf{J}$ is the Jacobian matrix. We solve the linearized system by using GMRES, one kind of Krylov subspace methods for nonsymmetric matrices. Since the method suffers from slow convergence, preconditioning is needed in conjunction with GMRES.

Fig. 5 shows the velocity vector of cavity flow test problem of a fluid with kinematic viscosity $\nu = 0.01\ m^2/s$ ($\rho = 1000\ kg/m^3,\ \mu = 10\ kg/ms$), $Re = 2$, using DSD/SST-SUPS formulation at time $t = 1000\Delta t$ where $\Delta t = 0.002$. The numerical test was conducted on a fixed $[0,1] \times [0,1]$ domain.

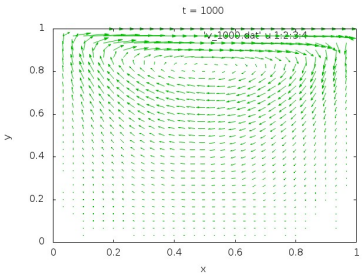

Fig.5 velocity vector of cavity flow at time $t = 1000\Delta t$

Finally, we couple interface-network and fluid models. Numerically, this is a weak coupling where the interface model and fluid model are solved independently for each time step., as in the following algorithm:
Repeat for $n = 0, 1, ...$

- Run one step of the interface model with current pressure p as outer force to get the interface position at t_{n+1}. We minimize the functional

$$\tilde{F}_n(\mathbf{u}) = F_n(\mathbf{u}) + \int_\Omega \frac{\mathbf{f}\cdot\mathbf{u}}{\sqrt{4\pi n h}},$$

where

$$\mathbf{f}(x) = \begin{cases} p\dfrac{(\boldsymbol{p}_i\cdot\boldsymbol{p}_j - 1)}{|\boldsymbol{p}_i - \boldsymbol{p}_j|^2}(\boldsymbol{p}_i - \boldsymbol{p}_j), & \text{if} \quad \text{dist}(x,\gamma_k) < \delta_1, \\ & \qquad\quad \text{dist}(x,P_k) > \delta_2 \\ \mathbf{0}, \quad \text{otherwise} \end{cases}$$

Here, $\gamma_k, k \neq i, j$ is the interface between phase P_i and P_j. δ_1, δ_2 are small positive constants, p is pressure, $\boldsymbol{p}_i, \boldsymbol{p}_j$ are the BMO reference vectors.

- Using the information of interface position at t_n and t_{n+1}, determine the domain occupied by fluid and run one step of the fluid model to obtain velocity and pressure of fluids at t_{n+1}.

In this coupling problem, we have separate mesh for interface and fluid model. The mesh for interface does not change during simulation but the fluid mesh changes as the interfaces change for each time step. To move the nodal points of fluid mesh, we use a kind of an automatic mesh moving scheme where the displacement of internal nodes is determined by solving elasticity equation. The coupling algorithm is depicted in Fig. 6.

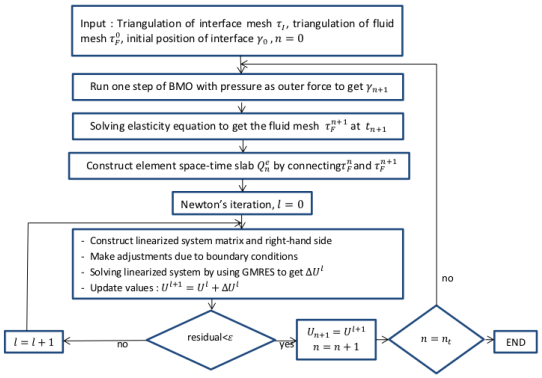

Fig.6 Numerical algorithm for coupled model

As a coupling example, we simulate bubble motion with buoyant force from the fluid in two settings, $\theta = 60°$ and $\theta = 120.1°$. Under the same buoyant force, we see that for a large contact angle ($\theta = 120.1°$), the bubble detaches from the bottom phase, while for $\theta = 60°$ the bubble remains attached (Fig.7).

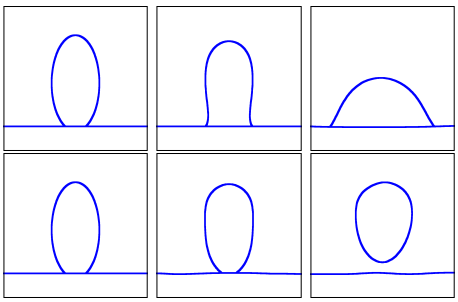

Fig.7 Bubble motion with $\theta = 60°$ ($\uparrow$, $\Delta t = 0.005$) and $\theta = 120.1°$ ($\downarrow$, $\Delta t = 0.001$)

The coupling result in this example is still in progress. We tried to figure out how to treat correctly the moving contact line which is, in conjunction with coupled problem, not an easy task. Here, we show one-way coupling examples in hydrophilic drop and hydrophobic drop cases as depicted in Fig.8

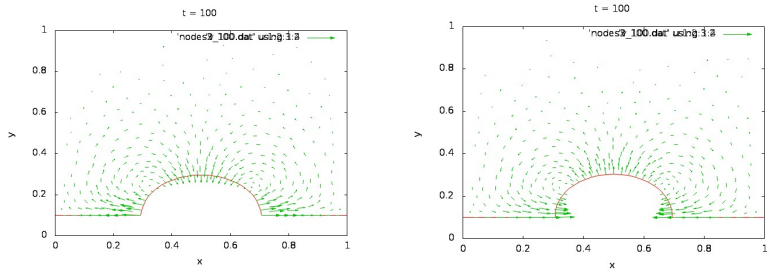

Fig.8(a) Hydrophilic drop case (b) Hydrophobic drop case

平成２６年８月４日

学位論文審査報告書（甲）

１．学位論文題目（外国語の場合は和訳を付けること。）

Simulation of Triple Line Dynamics by Interface-Fluid Coupling

界面と流体の連成による三重線ダイナミックスのシミュレーション

２．論文提出者　(1) 所　　属　数物科学　　専攻

(2) 氏（ふり）　名（がな）　Nur Shofianah（ヌル ショフィアナ）

３．審査結果の要旨（600～650字）

液滴の固体上の運動や多相流などで現れる三重線のダイナミックスは自然現象で重要な役割を持つが、その物理的な背景がまだ十分に理解されていない。現在では、三重線運動における要因の数理解析による理解に期待が寄せられている。Nur Shofianah氏は数理解析の土台となる三重線ダイナミックスのモデルを構成し、その数値実装を行うソフトウェアライブラリを構築した。本モデルは表面エネルギーの勾配流に基づく界面運動と Navier-Stokes 方程式による流体運動を採用しているシンプルな連成モデルであるが、界面の慣性や接触角のヒステレシスなどを含むより正確なモデルへの拡張の可能性を視野に入れている。このモデルにおいて、表面張力の異なる界面が交わる接合点の動きを再現することが一番の課題となる。Nur Shofianah氏はBMOアルゴリズムのアイデアを利用して、このような非対称な接合点の運動を求める数値解法を導出し、その正しさを数値結果の分析により確認した。さらに、時間とともに変形する2次元空間領域におけるNavier-Stokes方程式を時空における有限要素法を用いて数値的に解くプログラムを作成し、界面の運動と連成させたソフトウェアを開発した。以上の結果は数値シミュレーションによる三重線ダイナミックスの解析の基礎をなすという意味でこの分野への重要な貢献であると言える。以上により、平成２６年８月１日開催された公聴会に引き続き行われた審査会において、本論文は博士（理学）の学位を授与するに相応しいと判断した。

４．審査結果　(1) 判　　定（いずれかに○印）　(合　格)　・　不合格

(2) 授与学位　博　士（　理学　）