Numerical Analysis of Multiphase Curvature-driven Interface Evolution with Volume Constraint

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(体積保存条件を満たす複数の界面の曲率による運動の数理解析)

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Abstract

The dissertation focuses on two main points. First, we develop a signed distance vector approach for approximating volume-preserving mean curvature motions of interfaces separating multiple phase regions – a variant of the MBO (Merriman-Bence-Osher) threshold dynamics. We construct a vector-valued analogue of the signed distance function, which provides the needed subgrid accuracy on uniform grids without adaptive refinement; thereby, alleviating the well-known MBO time and grid restrictions. We adopt a variational method employing the idea of a vector-type discrete Morse flow, which allows us to easily treat volume constraint via penalization, and even, extend our method to include space-dependent bulk energies and anisotropic energies. We present several numerical tests and computational examples of curvature-driven interface evolutions.

Second, we analyze a penalization method related to the above volume-constrained variational problem – an approximation method that penalizes only the increase in volume. We present existence and regularity results of the sequence of minimizers of the corresponding penalized functional. Without relying on the smoothness of the free boundary, we investigate the behavior of these minimizers for sufficiently large penalty values. Lastly, we prove the existence of a minimizing movement corresponding to our penalized functional and some of its properties.

Consider a collection $\Gamma := \bigcup\{\gamma_{ij} : i, j = 1, 2, \ldots, k\}$ of hypersurfaces in $\mathbb{R}^N$, which partitions $\mathbb{R}^N = P_1 \cup P_2 \cup \cdots \cup P_k$ into k phase regions $P_i \subset \mathbb{R}^N$. Here, $\gamma_{ij} = \gamma_{ji}$ denotes the interface between P_i and P_j. The objective is to find a family $\{\Gamma(t) := \bigcup \gamma_{ij}(t)\}$ depending on time t such that every point $x \in \gamma_{ij}(t)$ moves with a velocity equal to a function of its mean curvature κ. To approximate such motions, we introduce a signed distance vector (SDV) approach based on a vector formulation of BMO (Bence-Merriman-Osher) threshold dynamics. We construct a vector analogue of the signed distance function, denoted by $\boldsymbol{\delta_\varepsilon} : \mathbb{R}^N \to \mathbb{R}^{k-1}$ and defined as follows: for $\varepsilon > 0$,

$$\boldsymbol{\delta_\varepsilon}(x) := \sum_{i=1}^{k} \left[1 - \min\left(1, \frac{dist\,(x, P_i)}{\varepsilon}\right)\right] \mathbf{p}_i,$$

where $\mathbf{p}_i$ is unit $(k-1)$-vector pointing from the centroid of a standard k-simplex to its vertex. With $\boldsymbol{\delta_\varepsilon}$ as an initial condition, we solve the vector-valued heat equation until time Δt. Then, for each x, identify the reference vector $\mathbf{p}_i$ closest to the solution $\mathbf{u}(\Delta t, x)$, that is,

$$\mathbf{p}_i \cdot \mathbf{u}(\Delta t, x) = \max_{j=1,2,\ldots,k} \mathbf{p}_j \cdot \mathbf{u}(\Delta t, x).$$

This redistribution of reference vectors determines the approximate new phase regions after time Δt, which defines $\Gamma(\Delta t)$. We formally show that SDV method evolves interface Γ with a normal velocity

$$v(x) = -\kappa + O(\Delta t), \quad \text{as } \Delta t \to 0.$$

Under this pure mean curvature motion, interfaces contract smoothly to enclose zero phase volume in finite time. We also establish the stability of triple junction as follows. Let $(\widehat{\theta}_1, \widehat{\theta}_2)$ be the junction angles after time Δt, then we can find a 2×2 matrix M whose largest singular value $\sigma < 1$ such that

$$\begin{bmatrix} \widehat{\theta}_1 - \frac{\pi}{3} \\ \widehat{\theta}_2 - \frac{\pi}{3} \end{bmatrix} = M \begin{bmatrix} \theta_1 - \frac{\pi}{3} \\ \theta_2 - \frac{\pi}{3} \end{bmatrix} + O(\delta^2 + \sqrt{\Delta t}), \quad \text{as } \Delta t \to 0,$$

where (θ_1, θ_2) denotes the initial junction angles and $\delta = \max(\theta_1 - \frac{\pi}{3}, \theta_2 - \frac{\pi}{3})$. This guarantees that at every time step of SDV algorithm, junction angles that are initially close to the symmetric configuration will always tend to get closer to 120° with an error of order $\sqrt{\Delta t}$; thus, stably imposing the symmetric Herring condition at the triple junction. Moreover, the classic shrinking circle test for mean curvature flow (MCF) reveals that SDV method alleviates the well-known BMO time and grid restrictions without mesh refinement – a clear advantage over its predecessors. Even with $\varepsilon = \Delta x$, our method does not stagnate, hence, saving computational costs.

Volume-constrained motions can also be realized using our method. We adopt a variational approach to solve the vector-valued heat equation based on the idea of discrete Morse flow and treat volume constraints via penalization as follows. Discretize $\Delta t = h \times K$. For a small positive number ϱ, successively minimize $(n = 1, 2, \ldots, K)$:

$$\mathcal{F}_n^h(\mathbf{u}) = \int_\Omega \left(\frac{|\mathbf{u} - \mathbf{u}_{n-1}|^2}{2h} + \frac{|\nabla \mathbf{u}|^2}{2} \right) dx + \frac{1}{\varrho} \sum_{i=1}^{k} \left| \omega_i - \mathcal{L}^N(P_i(\mathbf{u})) \right|^2,$$

where V_i denotes the prescribed volume of phase P_i, $\mathcal{L}^N$ denotes the N-dimensional Lebesgue measure, and

$$P_i(\mathbf{u}) := \{x \in \Omega : \mathbf{p}_i \cdot \mathbf{u}(x) \geq \mathbf{p}_j \cdot \mathbf{u}(x),\ \forall j = 1, 2, ..., k\},$$

the set corresponding to phase P_i with respect to solution $\mathbf{u}$. Figure 1 depicts the volume-preserving mean curvature evolution of an initial 10-phase configuration with circular arcs. We see that our method naturally handles topological changes, evident from the junction-junction collision at time $t = 133\Delta t$. Observe also that the symmetric junction angle conditions are satisfied and phase volumes are well-preserved.

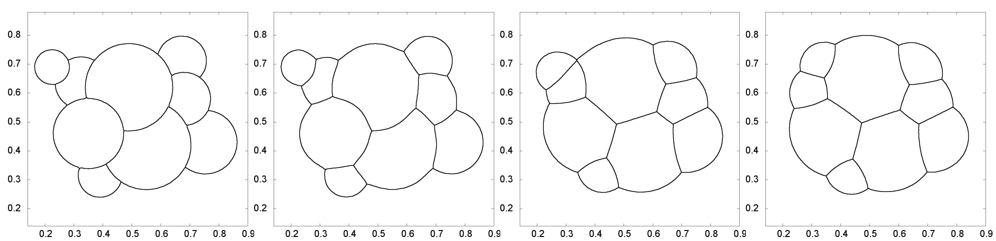

Figure 1: Initial 10-phase configuration; its SDV evolution after one time step $\Delta t = 2.5 \times 10^{-4}$; at time $t = 133\Delta t$ when a quadruple junction appears; and its stationary solution under penalty $\varrho = 10^{-6}$.

Our method can also be extended to a more general case where each phase region P_i has prescribed space-dependent bulk energy density e_i. We apply the SDV process to the vector-valued nonhomogenous heat equation $\mathbf{u}_t(t, x) = \Delta \mathbf{u}(t, x) + \mathbf{w}(x)$. If $\mathbf{w} \cdot (\mathbf{p}_i - \mathbf{p}_j)$ is bounded in $\mathbb{R}^N$ and

$$\mathbf{w}(x) \cdot (\mathbf{p}_i - \mathbf{p}_j) = \frac{k}{\varepsilon(k-1)} (e_i - e_j),$$

then the normal velocity of γ_{ij} at x is given by

$$v(x) = -\kappa - e_i + e_j + O(\Delta t), \quad \text{as } \Delta t \to 0.$$

We applied this method to simulate multiple rising gas bubbles in a liquid-filled container. In this setup, gas bubbles have zero bulk energies, while the liquid bulk energy density is given by $f = \beta y$ where β is a constant expressing buoyancy and y is coordinate direction of gravity. Here, we incorporate the influence of pressure force in the parabolic framework, where the bulk energy can be interpreted as an energy potential. Figure 2 shows that the volume-constrained evolution of interfaces using our method. The resulting motion of the two phase regions initially attached to the boundary floor is a contest between the buoyant force pushing the bubbles upwards and the surface tension force holding the bubbles down. Meanwhile, the volume difference in the right double bubble is greater than that of the left double bubble, causing it to turn and rotate faster than its counterpart and resulting in the merging of the two double bubbles.

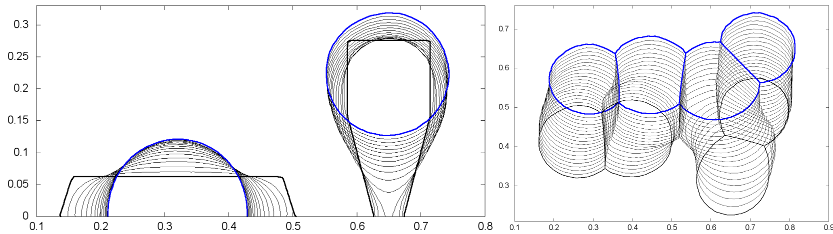

Figure 2: Evolution of interfaces initially attached to the boundary floor (left) and merging of two double bubbles (right) under parameters $\Delta t = 10^{-3}$, $\varrho = 10^{-5}$, and $f = 25y$.

To approximate two-phase anisotropic mean curvature evolution, we successively minimize the functional for $n = 1, 2, \ldots, K$

$$\mathcal{J}_n^{h,\phi}(u) = \int_\Omega \left(\frac{|u - u_{n-1}|^2}{2h} + \frac{|\phi(\nabla u)|^2}{2} \right) dx,$$

where $u_0 = \delta_\varepsilon$, time step size $\Delta t = h \times K$, and ϕ is the prescribed anisotropy function. Compared to its BMO counterpart, our method proceeds the evolution without stagnation. In the multiphase case, however, the evolution of the interface network near the junction is not correctly realized since our scheme only imposes the symmetric angle conditions. Hence, some form of nonsymmetric reference vectors in conjunction with our signed distance vector may be adopted to get a closer approximation of the junction evolution. We end with some computational examples of a two-phase mean curvature motion driven by different anisotropic energies using our method.

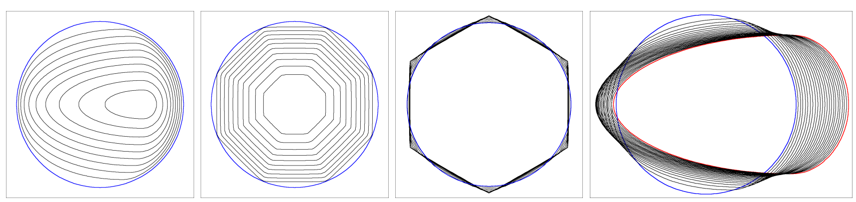

Figure 3: Examples of anisotropic mean curvature evolution of a circle with and without volume constraint generated via SDV method.

Next, we shift our attention to a penalization method for an evolutionary free boundary problem with volume constraint. Let $\Omega \subset \mathbb{R}^N$ be an open bounded connected domain with smooth convex Lipschitz boundary. Consider a nonnegative Lipschitz continuous function $u_0 \in H^1(\Omega) \cap L^\infty(\Omega)$ whose set of positive values has Lebesgue measure $\alpha \in (0, |\Omega|)$. Given time step $h = T/M$ for some fixed time $T \in (0, \infty)$ and $M \in \mathbb{N}$, we search for a sequence of functions $u_n \in H^1(\Omega)$ by successively solving the following problem for $n = 1, 2, \ldots, M$,

$$\begin{cases} u_n = \arg\min\limits_{\mathcal{A}} \displaystyle\int_\Omega \left(\frac{|u - u_{n-1}|^2}{h} + |\nabla u|^2 \right) dx \\ \mathcal{A} := \left\{ u \in H^1(\Omega) : \ |\{u > 0\}| = \alpha \right\}. \end{cases}$$

To solve this problem, we use an approximation method that penalizes only the increase in measure of the set $\{u > 0\}$. For a penalty parameter $\lambda > 0$, define functional

$$\mathcal{F}(h, u, u_{n-1}) = \mathcal{F}_n^h(u) := \int_\Omega \frac{|u - u_{n-1}|^2}{h} + |\nabla u|^2 + \lambda f(|\{u > 0\}|),$$

where the penalization function $f(x) = (x - \alpha)_+$. Consider the problem of successively minimizing the above functional for $n = 1, 2, \ldots, M$,

$$\min_{u \in H^1(\Omega)} \mathcal{F}(h, u, u_{n-1}).$$

We first show the existence of a sequence of minimizers u_n of functional $\mathcal{F}_n^h$. Note that u_n is bounded by the L^∞-norm of the initial condition u_0. To wit, $0 \le u_n \le \|u_0\|_{L^\infty(\Omega)}$. In addition, u_n is locally Hölder continuous in Ω and satisfies (in the weak sense)

$$\Delta u_n = \frac{u_n - u_{n-1}}{h} \quad \text{in } \{u_n > 0\}.$$

This allowed us to establish that the measure of $\{u_n > 0\}$ is never less than the prescribed measure. In particular,

$$\alpha \le |\{u_n > 0\}| \le \alpha + \lambda^{-1} \|\nabla u_0\|^2_{L^2(\Omega)},$$

which implies that $|\{u_n > 0\}| = \alpha$, as penalty value λ increases without bound. Invoking the Hölder continuity of the minimizers u_n (under the assumption that also $u_0 \in C^{0,\gamma}_{loc}(\Omega)$), we can show that u_n is locally Lipschitz continuous – a stronger regularity. Further, we establish the regularity of minimizer u_n up to the fixed Neumann boundary. Without relying on the smoothness of the free boundary, we study the behavior of minimizer u_n of $\mathcal{F}_n^h$ for sufficiently large penalty parameter λ. In particular, we see that we can take λ large enough that the measure of the set $\{u_n > 0\}$ adjusts to the prescribed value α. As a consequence, the solution to the original problem is attained without having to take λ to infinity. Finally, we construct a minimizing movement u associated to functional $\mathcal{F}$ in $L^2(\Omega)$ and initial datum u_0 and some of its properties, which includes Hölder continuity, more precisely, $u \in C^{0,1/2}([0, +\infty], L^2(\Omega))$.

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。）

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体積保存条件を満たす複数の界面の曲率による運動の数理解析

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３．審査結果の要旨（600～650字）

平均曲率流による界面運動は数多くの自然現象のモデルに現れ、応用上で重要な問題である。最近では特に接合点を含む界面ネットワークの動き、そして界面の囲う相の体積が保存されるなどの条件がつく動きが注目されている。Mohammad 氏は接合点を含む体積保存平均曲率流の効率的な数値解法を提案し、その理論的な裏づけを行った。位相変化にも対応できるレベルセット法に基づいた近似法が既に開発されているが、格子を細かくしない限り界面が停滞してしまう欠点があり、それぞれの相の体積が保存される条件の実現方法が知られていなかった。Mohammad 氏は符号つき距離関数のベクトル版を定義し、それをベクトル値に拡張された BMO アルゴリズムに導入することにより格子の分割数に対する制約をなくすことに成功した。また、このように改良されたアルゴリズムの形式的な解析により、接合点の角度が Herring 条件を満たす平均曲率流に収束することを示した。さらに、アルゴリズムで使われる偏微分方程式を変分法に持ち込むことにより、体積保存をペナルティーの形で組み込むことを可能にした。時間半離散化された問題の場合、このペナルティーによる近似の数学解析を行い、ペナルティー係数が十分小さければ体積が保存されるという数値計算にとって重要な結果を得た。以上の結果は界面ネットワークの幾何学的運動の数値計算と数学的な理解に大きく貢献している結果である。以上により、平成２６年８月１日開催された公聴会と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　）