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On Tracking Free Surfaces in Liquids

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Abstract: We consider a variational principle suitable for tracking boundaries of gas bubbles in liquids and its consequences. The principle is derived from a generalization of the *Principle of Stationary Action* applied to a Riemannian manifold of volume preserving flow maps. The dual variational principle for the markers tracking the free surfaces is induced by the Wasserstein-Kantorovich metric. This later variational principle provides means to compute the dynamics of free, implicit, surfaces without explicitly solving for the fields and quantities which define them. The presented theory suggests the following *approximate* evolution equation for the characteristic function of the gas, written in the Lagrangian frame of reference,

$$\begin{aligned}&\rho_G\left(\partial_{tt}\chi(\boldsymbol{x},t)-\lambda\partial_t\chi(\boldsymbol{x},t)\right)=\operatorname{div}\left(\chi(\boldsymbol{x},t)\left(\left(\rho_G-\rho_L\right)\vec{g}+\alpha\nabla H(\boldsymbol{x},t)\right)\right),\\&\boldsymbol{x}\in S(\nabla\chi),\quad t>0,\end{aligned}$$

where $S(\nabla\chi)$ represents the set of points on the gas-liquid interfaces, and H denotes the mean curvature of the interface. The constants α and λ denote the surface tension and Rayleigh's friction dissipation constants, respectively. The density of the liquid and gas are denoted ρ_L and ρ_G. The gravitational force is denoted $\vec{g}$. The regularized version of this equation is given, for some $\epsilon>0$, by

$$\begin{aligned}&\rho_G\left(\partial_{tt}s_\epsilon(\boldsymbol{x},t)-\lambda\partial_t s_\epsilon(\boldsymbol{x},t)\right)\\&=\operatorname{div}\left(s_\epsilon(\boldsymbol{x},t)\left(\left(\rho_G-\rho_L\right)\vec{g}+\nabla\left(\tfrac{2\alpha_0}{\epsilon}DW(s_\epsilon(\boldsymbol{x},t))-2\alpha_0\epsilon\,\Delta\, s_\epsilon(\boldsymbol{x},t)\right)\right)\right),\quad \boldsymbol{x}\in\Omega,\quad t>0,\\&DW(s)=s(1-s)(1-2s),\quad\text{and}\quad\alpha_0=3\alpha.\end{aligned}\tag{1}$$

Key Words: Free-boundaries, Navier-Stokes equations, $\Gamma-$convergence, Tracking.

1 Introduction

We offer an alternative to the transport equation for tracking free surfaces in liquids. When carefully interpreted, the equation we present allows to compute the evolution of the free boundaries without simultaneously solving for the velocity field or the pressure. The situation we strive to handle is associated with tracking the boundaries of a large number of possibly coalescing gas bubbles.

We consider a domain $\Omega \in \mathbb{R}^2$ containing two fluids which are supposed to be immiscible and incompressible, one of them being a gas. We assume that the gas is formed of bubbles. The incompressibility of bubbles is a reasonable hypothesis when the velocity of the bubble is small with respect to the velocity of sound in the gas contained in it. In this case, any local perturbation of the pressure occurring in the gas is almost instantaneously transmitted. This means that the gas essentially reacts as an incompressible fluid. We assume that the two fluids, submitted to gravitation and the action of surface tension, are separately governed by incompressible Euler equations. However, we add to this evolution system a Rayleigh's friction dissipative term, similar to the dissipative term of classical mechanics, [19], which is proportional to the velocity field. In other words, compared to the standard form of the Navier-Stokes equation, we assume that the spectrum corresponding to the Laplacian of the velocity is narrow, and that it can be "well" represented by a single number $-\lambda$, where $\lambda > 0$. This assumption has been introduced in [15].

It is known, [2], that the Euler equations are governed by the Least Action Principle on the configuration space of incompressible, one-to-one and onto flow maps. This means that the flow maps given by the Euler equations are geodesic curves on this space with respect to the L^2-Riemannian metric, [5], defined by the kinetic energy. It seems that no such principle is available for the dissipative flows. Since we need, as a starting point, a variational principle, we modify PSA. The modification consists in the introduction of the weighting factor $e^{\lambda(t-t_0)}$ in the definition of the Action. We show that the dissipative flows (with the Rayleigh's friction dissipative term) are indeed governed by such a generalization of the Least Action Principle.

Our approach is based on a sequence of variational problems. The different steps are as follows.

1. A variational principle for the flow maps governed by the Euler equations with the added dissipative friction term.

2. Semi-discretization in time of the Lagrangian yielding a variational problem for the update of the flow maps. The scheme provides naturally the variational formulation of the implicit Euler time stepping scheme applied to the evolution system. The corresponding "dual" variational formulation is based on the Wasserstein metric for the semidiscretized characteristic function, the Indicatrix (that we occasionally call "marker function").

3. The $\Gamma-$regularization of the variational formulation for the Indicatrix. The implicit time stepping scheme for the regularized Indicatrix is obtained by approximating the Gâteaux derivative of the regularized variational problem.

4. Taking an appropriate limit as $\triangle t \to 0_+$ to obtain a time continuous equation.

5. Taking the Γ-limit as $\epsilon \to 0_+$ to remove the regularization.

Obtaining a variational principle for the underlying evolution equations is a crucial step. It allows us to reduce the update in time of the flow maps to a variational problem instead of solving a semidiscretized form of the evolution system. This idea is introduced and explored by F. Otto in [11], [18], [8]. In [18], an approach similar to the outlined program has been used, though with averaging as a focal point, to model evolution of the Hele-Shaw flows. The importance of the semidiscretization of the variational principle for the flow maps is in that it introduces a metric on the space of the characteristic functions, i.e., a topology, that turns out to be the Wasserstein-Kantorovich distance. Another important ingredient of the variational approach is how to obtain a smooth approximation to the Indicatrix, which has values only 0 or 1. The Lagrangian describing the system belongs to the class of Mumford-Shah functionals. This classification leads to the $\Gamma-$regularization of the Lagrangian, which relaxes the nonconvex 0/1 identification of the compounds, as well as it provides a coarse grained model of the coalescence. This communication is based on extension of [10], which does not include a finite element discretization we propose for the unusual forth-order problem presented here, [4], and which does not include numerical simulations, [9].

2 Dissipative Flow Maps

Let the Eulerian Indicatrix function $\chi \in BV(\Omega, \{0,1\})$ represent the characteristic function of the domain Ω_G occupied by the gas. We set $\chi(\vec{x},t) = 1$ for $\vec{x} \in \Omega_G$ and $\chi(\vec{x},t) = 0$ otherwise. The Indicatrix χ tells us if, at some time t, the point $\vec{x}$ represents a liquid or gas. In terms of the Lagrangian description, we can achieve similar identification by considering a flow map $\vec{X}(\vec{x},t)$ which provides the location at a time t of the particle which was at the point $\vec{x}$ at time $t = t_0$. We assume that for each time t, $\vec{X}(\cdot,t)$ is a one-to-one and onto map $\Omega \mapsto \Omega$. Since we consider incompressible fluids, we further require any $\vec{X}$ to be volume preserving. We assume that the flow maps are separately smooth both in Ω_G and in $\Omega_L = \Omega \backslash \Omega_G$ for any $t > 0$. The Lagrangian of our system includes the kinetic, potential, and surface energies. Since both densities are constant, we have

$$\rho_0(\boldsymbol{x}) \stackrel{\text{def}}{=} \rho(\vec{x},0) = \rho(\vec{X}(\boldsymbol{x},t),t).$$

We assume that the density ρ is given by

$$\begin{aligned}&\rho(\vec{X}(\vec{x},t),t)\\ &= \rho_G \chi(\vec{X}(\vec{x},t),t) + \rho_L(1-\chi(\vec{X}(\vec{x},t),t)),\end{aligned}$$

where ρ_G, ρ_L are the density of the gas and liquid, respectively. We consider a gas-liquid system with the Lagrangian of a Mumford-Shah type, [16], given by

$$\mathcal{E}(\vec{X},t) \stackrel{\text{def}}{=} \tfrac{1}{2} \int_\Omega \rho_0(\boldsymbol{x}) \left(\frac{d}{dt}\vec{X}(\boldsymbol{x},t)\right)^2 dx + E(\vec{X},t),$$

where

$$E(\vec{X},t) \stackrel{\text{def}}{=} \int_\Omega \rho_0(\vec{x})\, \vec{g} \cdot \vec{X}(\vec{x},t)\, dx + \alpha \left\|\nabla \chi(\cdot,t)\right\|(\Omega),$$

$$\chi\left(\vec{X}(\vec{x},t),t\right) = \chi(\vec{x},0).$$

The surface energy, $\alpha \left\|\nabla \chi(\cdot,t)\right\|(\Omega)$, i.e., the total variation of $\nabla\chi$, represents the perimeters of the subdomains occupied by the gas multiplied by a surface tension coefficient α which is a positive measured quantity. The vector $\vec{g}$ represents the gravitation force field.

We apply a generalization of the *Principle of Stationary Action*, PSA, [12], to the above Lagrangian in order to ensure that the underlying dynamics are indeed given by the Euler equations with the added dissipative term, and to show that the pressure drop across the gas-liquid interfaces satisfies the Laplace-Young equation. We omit details here. To account for the dissipative effects, we define the action as

$$A(\vec{X},t_1,t_2) \stackrel{\text{def}}{=} \int_{t_1}^{t_2} e^{\lambda(t-t_0)} \mathcal{E}(\vec{X},t)\, dt,$$

where $\lambda > 0$ represents the Rayleigh's friction dissipation coefficient, and $t_0 \geq 0$ is a given initial time. Then

$$\vec{X} \mapsto A(\vec{X},t_1,t_2)$$

represents a functional on the *configuration space* $\mathcal{M}$. We require the action to be stable on the flow maps $\vec{X}(.,t) \in \mathcal{M}$ with respect to variations which are compatible with the incompressibility and the immiscibility constraints. Therefore we consider a family of maps $\vec{X}_\tau$ preserving the Lebesgue measure such that $\vec{X}|_{\tau=0} = \vec{X}$. We set

$$\vec{Y} = \frac{d}{d\tau}\vec{X}_\tau\big|_{\tau=0}.$$

Hence, $\vec{Y} \in T_{\vec{X}(.,t)}\mathcal{M}$. We implement the Principle of Stationary Action by requiring the Gâteaux derivative of the action to vanish on variations $\vec{Y} \in T_{\vec{X}(.,t)}\mathcal{M}$ satisfying $\vec{Y}(.,t_1) = \vec{Y}(.,t_2) = 0$, i.e., the weakly dissipative Navier-Stokes equations are given by

$$dA(\vec{X},t_1,t_2,\vec{Y}) = 0, \text{ for all } \vec{Y}(.,t) \in T_{\vec{X}(.,t)}\mathcal{M}.$$

3 Monge-Ampère Transport

Let $\tau_k = k\,\Delta\tau$, and let $\vec{X}^k(.) \stackrel{\text{def}}{=} \vec{X}(.,k\,\Delta\tau)$. In accordance with the (G)PSA, we assume that for given maps $\vec{X}^0$, $\vec{X}^n$ the maps $\vec{X}^k$, $k = 1,\ldots,n-1$, $n \geq 1$, are obtained by the variational principle

$$\left\{\vec{X}^k\right\}_{k=1}^n \stackrel{\text{def}}{=} \underset{\vec{Y}^1,\ldots,\vec{Y}^n \in \mathcal{M}}{\text{Arginf}} \mathcal{L}_k, \qquad \text{where} \tag{2}$$

$$\begin{aligned}\mathcal{L}_k \stackrel{\text{def}}{=} &\sum_{k=1}^n \tfrac{1}{2} \int_\Omega \rho_0(\boldsymbol{x}) \left|\vec{Y}^k - \vec{Y}^{k-1}\right|^2 (\lambda t_k + 1)^2\, dx\\ &+ \sum_{k=1}^n (\Delta t_k)^2\, E(\vec{Y}^k).\end{aligned}$$

In other words, the Lagrangian flow maps $\vec{X}^k$ are a time discrete solutions of the Navier-Stokes equations. Our purpose is to show that we can

reformulate the above variational principle as a Monge-Ampère transport problem that leads to a variational principle for the Indicatrix using the Wasserstein metric. As the first step in this direction, we have

Theorem 1 *Let us assume that Ω is bounded with piece-wise smooth boundary. Let us assume that χ^0 and $\chi^n \in \mathcal{K}$ are given, where $\mathcal{K}$ is a subset of $BV(\Omega, \{0,1\})$-markers that can be obtained from a given fixed initial χ^0 by a volume preserving map. Then there exist minimizers $\chi^1, ..., \chi^{n-1} \in \mathcal{K}$ of the following variational problem*

$$\inf_{\mathcal{K}} \sum_{k=1}^{n} \mathcal{D}_W \left(\tilde{\chi}^k, \tilde{\chi}^{k-1}\right)^2 + \left(\triangle t_k\right)^2 E_E(\tilde{\chi}^k), \qquad (3)$$

where

$$\mathcal{D}_W \left(\chi^k, \chi^{k-1}\right)^2 \stackrel{def}{=}$$
$$\tfrac{1}{2}\rho_G \operatorname{dist}_W \left(\chi^k, \chi^{k-1}\right)^2 + \tfrac{1}{2}\rho_L \operatorname{dist}_W \left(1-\chi^k, 1-\chi^{k-1}\right)^2$$
$$E_E(\chi) \stackrel{def}{=} \int_\Omega \rho(\boldsymbol{x})\vec{g}\cdot\vec{x}\, dx + \alpha \left\|\nabla\chi\right\|(\Omega).$$

The symbol dist_W *denotes the Wasserstein metric, [18], [11], [3].*

Proof. For the proof see [10], Theorem 4.7. ■

Next we mention that the variational problem (3) is in fact a dual to the variational problem (2). Namely, we have

Theorem 2 *Let us assume that Ω is bounded with piece-wise smooth boundary. Let us assume that maps $\vec{X}^0, \vec{X}^n \in \mathcal{M}$ are given. Then there exists a unique minimizer $\left\{\vec{X}^k\right\}_{k=1}^{n-1} \in S(\Omega)^n$, where $S(\Omega)$ is the set of measure preserving maps, of the variational problem (2) that satisfies*

$$\int_\Omega f(\mathbf{x})\chi^k(\mathbf{x})\, d\mathbf{x} = \int_\Omega \chi^0(\mathbf{x}) f(\vec{X}^k(\boldsymbol{x}))d\mathbf{x},$$
$$\text{for } k = 1, ..., n-1 \quad \text{and for all } f \in C^0(\Omega),$$

and where $\{\chi^k\}_{k=1}^{n-1}$ is the unique minimizer of (3).

Proof. For the proof see [10], Theorem 4.16. ■

Theorem 2 implies that we can obtain time updates for the evolution of the phase markers χ^k by approximating (!) the Gâteaux derivative of the Wasserstein metric. We note that the flow maps $\vec{X}^k$ are still contained in (3) due to the optimality of the transport of the markers.

3.1 G-derivative of the W-metric

Let s^k be the $\Gamma-$regularization of the markers obtained by the Cahn-Hillard approach, [6], [13], [14], [1]. We have

Lemma 3 *Let $\vec{X}_\tau \in \mathcal{M}$ be a family of optimal maps bringing s^k onto s_τ given by*

$$\vec{X}_\tau(\boldsymbol{x}) = \vec{X}^{k,k+1}(\boldsymbol{x}) + \tau\left(\nabla f \circ \boldsymbol{h}\right)(\boldsymbol{x}), \qquad \textit{where}$$

$f \in W^{2,2}\left(\Omega, \mathbb{R}^1\right)$ is arbitrary but with invertible gradient, $\boldsymbol{h} = (\nabla f)^{-1} \circ \vec{Z} \circ \vec{X}^{k,k+1}$, and $\vec{Z} \in T_{Id}\mathcal{M}$ is given. Then, up to the order of $\mathcal{O}(\left\|D^2 f\right\|)$,

$$\frac{d}{d\tau}\frac{1}{2}\operatorname{dist}_W(s^k, s_\tau)^2\big|_{\tau=0}$$
$$\approx \int_\Omega f(\boldsymbol{x})\left(s^{k+1}(\boldsymbol{x}) - 2s^k(\boldsymbol{x}) + s^{k-1}(\boldsymbol{x})\right) dx$$
$$+ \int_\Omega f(\boldsymbol{x})\left(s^k(\boldsymbol{x}) - s^{k-1}(\boldsymbol{x})\right) dx$$
$$- \int_\Omega (\boldsymbol{h}(\boldsymbol{x}) - \boldsymbol{x})\cdot\nabla f(\boldsymbol{h}(\boldsymbol{x}))s^k(\boldsymbol{x})\, dx$$
$$+ \int_\Omega \left(\vec{X}^{k,k+1} - \boldsymbol{x}\right)\left(\left(\nabla f \circ \boldsymbol{h}\right)(\boldsymbol{x}) - \nabla f(\boldsymbol{h}(\boldsymbol{x}))\right) s^k\, dx.$$

Proof. For the proof see [10], Lemma 5.1. ■

With Lemma 3 at hand, after performing the remaining Gâteaux derivatives, and after rescaling back the time coordinate, we obtain an implicit time-discrete scheme for the regularized marker s obeying the equation (1). Details concerning the derivation of this equation can be found again in [10].

In the remainder of the communication, we address the space discretization of (1), which is a unusual fourth order problem, and we discuss some numerical results.

4 An approximation of markers

Well-known nonconforming finite element approximation of solutions to, say, the plate problems, such as Adini-Clogh-Melosh finite element and alikes, [7], proved in our particular setting counterproductive: initially sharp transition region (due to the Cahn-Hillard approximation of the phase boundary) soon dissipates, which produces adverse side-effects on the transient dynamics. The reason turns out to be the affect of

the viscosity term. We circumvent this problem by introducing non-conforming approximations on both the second-order (i.e., with respect to the Laplace operator), and fourth-order (i.e., biharmonic) levels. Namely, assuming $\Omega \subset \mathbb{R}^2$, we propose two different finite elements $\{Q, \Sigma, P_i\}$, $i = 1, 2$, $Q = (-1, 1)^2$, and where

$$P_1 \stackrel{\text{def}}{=} \text{Span}\{1, x, y, xy, x^2, y^2, x^2y, xy^2\},$$

$$P_2 \stackrel{\text{def}}{=} \text{Span}\{1, x, y, xy, x^2y, xy^2, x^2y^2, x^2 - y^2\},$$

$$\Sigma \stackrel{\text{def}}{=}$$

$$\text{Span}\left\{p(a_i), \int_{F_i} \nabla p(s) \cdot \vec{n}(s)\, dS \,|\, i = 1, \ldots, 4\right\}.$$

Here, a_i denote the vertices of Q, F_i denote the sides of ∂Q, $p \in P_i$, $i = 1, 2$, and dS denotes the invariant infinitesimal surface element. The underpinning analysis for these elements including convergence, error estimates and stability can be found in [4]. We note that the polynomial space P_2 is not affine: P_2 is not invariant under non-$SO(2)$ maps in view of the term $x^2 - y^2$.

5 A numerical simulation

We use the equation (1) to compute motion and subsequent coalescence of two gas bubbles. Simultaneously, we "compare" the numerical results with the novel approach for tracking bubbles in viscous fluid governed by the Navier-Stokes equations developed in [17]. We add to our dynamical system the following initial and boundary conditions

$$\begin{aligned} &s(\boldsymbol{x}, 0) = s^0(\boldsymbol{x}), && \boldsymbol{x} \in \Omega, \\ &\partial_t s(\boldsymbol{x}, 0) = -\vec{v}(\boldsymbol{x}, 0) \cdot \nabla s^0(\boldsymbol{x}), && \boldsymbol{x} \in \Omega, \\ &\nabla s(\boldsymbol{x}, t) \cdot \boldsymbol{n} = 0, && \text{on } \partial\Omega, \\ &s(\boldsymbol{x}, t) = 0, && \text{on } \partial\Omega. \end{aligned} \tag{4}$$

We take $v(\vec{.}, 0) = 0$, the regularized marker s^0 describes two bubbles positioned to coalesce in view of their unequal sizes due to the buoyant upward oriented force, c. f., Figure 1.

Rough comparison of the approaches is shown on the pictures below. The dark thick contour shows membrane of the regularized marker computed with (1), while the underlying numerical results were communicated to the author by M. Romerio, [17]. The results are both qualitatively and quantitatively different. Nevertheless they do show some similarities. There is a number of reasons for the differences: slightly different field model for the velocity, different treatment of the coalescence ($\Gamma-$regularization versus artificial creation of a new bubble based on a proximity condition used in [17]), different numerics, etc. We want to emphasize that the equation (1) is only a first order approximation due to a complicated form of the Gâteaux derivative of the Wasserstein metric. We only approximate this formula. One of the similarities we can agree upon is that both models can handle coalescence in one way or another including post-coalescence dynamics. Which of the two models (and of course of the ones we did not use for the comparison) is more true to the reality remains to be seen.

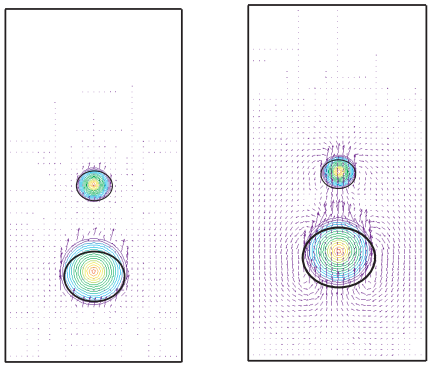

Figure 1: Pre-coalescence in a vertical channel.

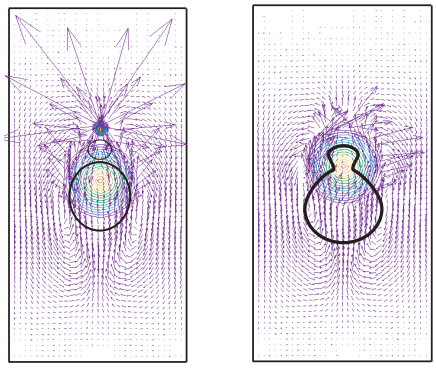

Figure 2: The moments of coalescence. Note the differences between the two models. The significant property of (1) is in a diffeomorphic shape transition due to the regularizing effects of the surface energy.

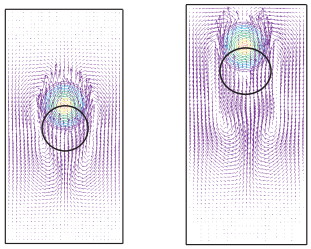

Figure 3: Post-coalescence dynamics. Note the slowdown predicted by the dynamical system (1).

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