Surfactant Dynamics from the Arnold perspective

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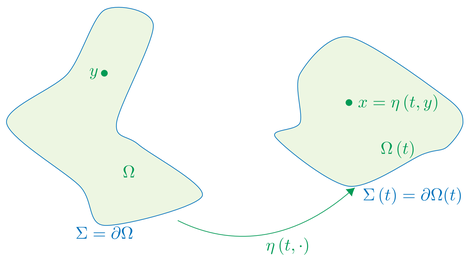
Motivation and Setup

Background/Abstract

Partial differential equations (PDEs) are an integral tool for modeling the world around us, as they accurately describe a huge array of natural phenomena, notably including the development of and long term behaviour of fluids. Consequently, the study and characterization of PDEs has held a prominent place in mathematics for centuries. However, despite their ubiquity, reasoning about solutions to these systems still remains incredibly difficult, with the behaviour of relatively simple systems remaining completely open. Although a number of different analytical tools have been developed in order to better study these systems, such as the theory of Sobolev spaces, an interesting new development has come from V. Arnold, who recently developed a new method for analyzing PDEs related to the Euler equations (which describe the behaviour of incompressible fluids). Using ideas from the calculus of variations, Arnold established an important connection between these equations and a set of geodesic flows, using variational techniques to characterize the latter as solutions to the former.

Motivated by his results, in this project, we investigate PDEs that characterize minimizers of energies related to surfactants, which are substances that adhere to fluids and have the ability to change quantities like surface tension. With notable examples including detergents, emulsifiers, and soap bubbles, the behavior of surfactants is of importance in the cosmetic industry, ore extraction and in biology, where they prevent the collapse of lungs during normal breathing. By careful choice of the different related energies, we rederive several of the classically known PDEs related to surfactants, while also deriving new systems that are of independent interest.

Setup and Notation



Throughout, our domain of interest will be a fixed open and connected subset of $\mathbb{R}^n$, which will serve as an initial reference frame for our fluid. Denoting this set by Ω, we then set $\Sigma := \partial\Omega$ to be it's boundary and $\nu : \Sigma \to \mathbb{R}^n$ to be the associated outward pointing unit normal.

Given any such domain, we can then define the function spaces $\mathrm{Diff}_0(\Omega), \mathrm{FDiff}(\Omega) \subseteq L^2(\Omega; \mathbb{R}^n)$, which are set to be

$$\mathrm{Diff}_0(\Omega) = \{\eta : \Omega \to \Omega \mid \eta \in \mathrm{FDiff}(\Omega)\}$$
$$\mathrm{FDiff}(\Omega) = \{\eta : \Omega \to \mathbb{R}^n \mid \eta \text{ a volume/orientation preserving diffeomorphism}\}.$$

Viewing such functions as possible states for the fluid, we see then that Diff_0 corresponds to the space of states where the fluid remains fixed inside Ω (so in particular the boundary remains the same), whereas FDiff is the space of states where the fluid can move around arbitrarily in $\mathbb{R}^n$, as depicted in the diagram above. In either case, we have that η provides Lagrangian coordinates for the fluid.
With these spaces defined, we note also a result from differential geometry which tells us that $\mathrm{FDiff}(\Omega)$ and $\mathrm{Diff}_0(\Omega)$ are smooth manifolds, with their respective tangent spaces at any point η satisfying

$$T_\eta \mathrm{Diff}_0(\Omega) = \{u \circ \eta \in L^2(\Omega; \mathbb{R}^n) \mid \mathbf{div}\ u = 0, u \cdot \nu = 0\} \tag{1}$$
$$T_\eta \mathrm{FDiff}(\Omega) = \{u \circ \eta \in L^2(\Omega; \mathbb{R}^n) \mid \mathbf{div}\ u = 0\} \tag{2}$$

Technical Tools

Existence of a Perturbation

With these preliminaries established, we'll now move onto various technical results, which will facilitate the calculations and constructions used to derive our final PDEs. To begin, consider the space X of all flows associated to Ω over the time interval $[0, 1]$; that is,

$$X := \{\eta \in C^1([0,1]; \mathrm{FDiff}(\Omega)) \mid \eta(0) = \eta_0, \eta(1) = \eta_1\}$$

where η_0, η_1 are some fixed initial and terminal states of the fluid. Given any $\eta \in X$, we can then view this function as a path between η_0 and η_1 along the manifold FDiff, with $\eta(t)$ encoding "where the fluid is at time t." Since we're then interested in characterizing *shortest* paths along FDiff, a natural question to then ask would be what local changes can be made to such a path η.
Fixing any such one-parameter family of flows $\zeta(s) : (-\varepsilon, \varepsilon) \to X$ with $\zeta(0) = \eta$, an obvious necessary condition is that $\partial_s \zeta(0)(t)$ is in the tangent space of FDiff at $\eta(t)$. Using techniques from the theory of ODE, we can show that this is also a sufficient condition; that is, given an arbitrary velocity field v_0, we can find ζ parametrizing perturbations of η such that the derivative of ζ at η is equal to the desired velocity field.

Formally, the statement is as follows.

***Lemma* 1.** *Let $v_0 : [0,1] \to \{v \in L^2(\Omega; \mathbb{R}^n) \mid \mathbf{div}\ (v \circ \eta^{-1}) = 0\}$, $\eta_0, \eta_1 \in \mathit{FDiff}(\Omega)$ be fixed. Then there exists a perturbation $\zeta : (-\varepsilon, \varepsilon) \to X$ such that:*

$$\zeta(0) = \eta, \zeta(s) \in C^\infty, \text{ and } \partial_s \zeta(x, 0, t) := v(\eta(x,t), 0, t) = v_0(\eta(x,t), t)$$

Using this lemma, since we now know that $\frac{d\zeta}{ds}$ can be specified arbitrarily, we obtain useful characterizations of local minima of the energies that we can use in conjunction with the following results.

Decompositions of L^2

Now with the previous result in hand, we consider different orthogonal decompositions of L^2, which will allow us to explicitly obtain formulae for functions that vanish when tested against the divergence free velocity fields above.
The first result we state is the Leray decomposition, which allows us to introduce the pressure term that will appear in our later PDEs.

***Theorem* 1** (Leray Decomposition). *Let $\mathcal{V}$ be the space of smooth and compactly supported divergence free functions; that is,*

$$\mathcal{V} = \{\varphi \in C_c^\infty(\Omega; \mathbb{R}^n) \mid \mathbf{div}\ \varphi = 0\} \tag{3}$$

Let H be the closure of $\mathcal{V}$ in $L^2(\Omega; \mathbb{R}^n)$. Then H and its orthogonal complement in $L^2(\Omega; \mathbb{R}^n)$ satisfy the following:

$$H = \{u \in L^2(\Omega; \mathbb{R}^n) \mid \mathbf{div}\ u = 0, u \cdot \nu = 0\} \tag{4}$$
$$H^\perp = \{\nabla p \in L^2(\Omega; \mathbb{R}^n) \mid p \in H^1(\Omega)\} \tag{5}$$

We also have an analogous result for functions that are not necessarily smooth:

***Theorem* 2.** *Let*

$$H' = \{u \in L^2(\Omega; \mathbb{R}^n) \mid \mathbf{div}\ u = 0\} \tag{6}$$

Then H' is a closed subspace of $L^2(\Omega; \mathbb{R}^n)$ and the orthogonal complement of H' in $L^2(\Omega; \mathbb{R}^n)$ is

$$H'^\perp = \{\nabla p \in L^2(\Omega; \mathbb{R}^n) \mid p \in H^1(\Omega), p = 0 \text{ on } \partial\Omega\} \tag{7}$$

Reynolds Transport Theorem on Hypersurfaces

The final result we will need is the Reynolds Transport Theorem, which is a result that allows us to obtain explicit formulae for the derivatives of boundary terms in our energies, which we will need for those energies involving surfactants.

***Theorem* 3.** *Let Σ be a hypersurface and $\beta \in C^1(\Sigma \times [0,1]; \mathbb{R}^n)$. Set $\Sigma(t) = \beta(\Sigma, t)$. If $f \in C^1(\mathbb{R}^n \times [0,1]; \mathbb{R}^n)$, then*

$$\frac{d}{dt}\int_{\Sigma(t)} f = \int_{\Sigma(t)} \partial_t f + \nabla f \cdot u + f \mathbf{div}_{\Sigma(t)} u \tag{8}$$

where $u(\beta(x,t),t) = \partial_t \beta(x,t)$ and the surface divergence is $\mathbf{div}_{\Sigma(t)} u = tr((I - \nu \otimes \nu) Du)$.

Main Results

Previous results: Arnold's setup

We start with Arnold's original derivation of the Euler equations, noting in particular the relative simplicity of the associated energy.

***Theorem* 4** (Arnold). *Let X_0 be the space of flows of Ω with fixed domain, i.e.*

$$X_0 := \{\eta \in C^1([0,1]; \mathit{Diff}_0(\Omega)) \mid \eta(0) = \eta_0, \eta(1) = \eta_1\}$$

where again η_0, η_1 are some fixed initial/terminal states. If they exist, minimizers of the energy functional $E : X \to \mathbb{R}^+$ defined via

$$E(\eta) = \int_0^1 \int_\Omega \frac{1}{2} |\partial_t \eta|^2 \, dx dt \tag{9}$$

satisfy the incompressible Euler equations with fixed boundary and uniform constant density; that is,

$$\begin{cases} \partial_t u + u \cdot \nabla u + \nabla p = 0 & \text{on } \Omega \\ \mathbf{div}\ u = 0 & \text{on } \Omega \\ u \cdot \nu = 0 & \text{on } \partial\Omega \end{cases} \tag{10}$$

where u is the Eulerian velocity defined via $u(\eta(x,t),t) = \partial_t \eta(x,t)$ and p is the pressure.

Proof Sketch. For any perturbation ζ as before, we know that we must have

$$\partial_s E(\zeta)\,|_{s=0} = 0$$

since $\zeta(0) = \eta$ is a minimizer. Now by considering arbitrary velocity fields as in the previous result, building corresponding perturbations, and expanding this out, we find that $\partial_t u + u \cdot \nabla u$ must vanish when tested against any smooth, compactly supported, and divergence free function. Using the Leray decomposition, we see that this term must be exactly the negative pressure gradient, which leads to the first equation. The second and third equations are then a consequence of the fact that η must be volume preserving and has fixed image. □

Result #1: Surface tension and potential

We now consider a significant complication of the Arnold functional, where we introduce a globally defined potential term φ (which can represent forces such as gravity or electromagnetism), allow the Eulerian and densities ρ of the fluid to vary over space, add a term σ to compensate for surface tension, and allow the fluid to move freely through space.

***Theorem* 5.** *Given a constant $\sigma \in \mathbb{R}^+$, $\overline{\rho} : \Omega \to \mathbb{R}^+$ and $\varphi \in C^1(\mathbb{R}^n)$, minimizers (if they exist) of the energy $E : X \to \mathbb{R}$ defined via*

$$E(\eta) = \int_0^1 \left(\int_\Omega \frac{\overline{\rho}}{2} |\partial_t \eta|^2 - \varphi(\eta)\, dx - \int_{\partial\Omega(t)} \sigma dS \right) dt \tag{11}$$

must satisfy the incompressible Euler equations with surface tension; that is,

$$\begin{cases} \rho(\partial_t u + u \cdot \nabla u) + \nabla p = -\nabla\varphi & \text{on } \Omega(t) \\ \mathbf{div}\ u = 0 & \text{on } \Omega(t) \\ p = -\sigma H & \text{on } \partial\Omega(t) \end{cases} \tag{12}$$

where $\Omega(t) := \eta(\Omega, t)$, u is the Eulerian velocity defined via $u(\eta(x,t),t) = \partial_t \eta(x,t)$, $\overline{\rho}, \rho$ are Lagrangian and Eulerian densities, and $H = -\mathbf{div}\ \nu$ is the mean curvature of $\partial\Omega(t)$.

Proof Sketch. We proceed as in the previous result. By first only considering compactly supported velocity fields, we can isolate the contribution of the terms defined on Ω to deduce the first equation. Considering general velocity fields, combining the Reynolds transport equation and the surface divergence theorem, and doing further computations then yields the other equations. □

Result #2 Penalizing surfactant boundary wiggling

Now we introduce a term to penalize the motion of surfactants that move alongside the boundary. Here the motion of the surfactants is determined by the motion of the flow map.

***Theorem* 6.** *Given $\overline{\rho} : \Omega \to \mathbb{R}^+$, $\xi : \mathbb{R} \to \mathbb{R}^+$, $\overline{\gamma}_0 : \partial\Omega \to \mathbb{R}^+$, $\varphi \in C^1(\mathbb{R}^n)$, let $E : X \to \mathbb{R}$ via*

$$E(\eta) = \int_0^1 \left(\int_\Omega \frac{\overline{\rho}}{2} |\partial_t \eta|^2 - \varphi(\eta)\, dx + \int_{\partial\Omega} \frac{\overline{\gamma}_0}{2} |\partial_t \eta|^2\, dS - \int_{\partial\Omega(t)} \xi(\gamma)\, dS \right) dt \tag{13}$$

with all relevant terms as defined above. Then minimizers (if they exist) of the energy functional E must satisfy

$$\begin{cases} \rho(\partial_t u + u \cdot \nabla u) + \nabla p = -\nabla\varphi & \text{on } \Omega(t) \\ \mathbf{div}\ u = 0 & \text{on } \Omega(t) \\ \gamma(\partial_t u + u \cdot \nabla u) - p\nu = \nabla_{\Sigma(t)}\sigma + H\nu\sigma & \text{on } \partial\Omega(t) \\ \partial_t \gamma + \nabla\gamma \cdot u + \gamma \mathbf{div}_{\Sigma(t)} u = 0 & \text{on } \partial\Omega(t) \end{cases} \tag{14}$$

where u is the Eulerian velocity, $\sigma = \xi(\gamma) - \xi'(\gamma)\gamma$ is the surface tension, $\overline{\rho}, \rho$ are densities, and p is the pressure term.

Result #3: Surfactants freely moving along boundary

Finally, we introduce another degree of freedom by allowing the surfactants to move along the boundary independently of the mass in the interior, as parameterized by a function β.

***Theorem* 7.** *Let X be as above and*

$$Y = \{\beta \in C^1([0,1]; \mathit{Diff}_0(\partial\Omega)) \mid \beta(0, x) = x\}$$

Given $\overline{\rho} : \Omega \to \mathbb{R}^+$, $\xi : \mathbb{R} \to \mathbb{R}^+$, $\overline{\gamma}_0 : \partial\Omega \to \mathbb{R}^+$, $\varphi \in C^1(\mathbb{R}^n)$, consider $E : X \times Y \to \mathbb{R}$ via

$$E(\eta, \beta) = \int_0^1 \left(\int_\Omega \frac{\overline{\rho}}{2} |\partial_t \eta|^2 - \varphi(\eta)\, dx + \int_{\partial\Omega} \frac{\overline{\gamma}_0}{2} |\partial_t (\eta \circ \beta)|^2\, dS - \int_{\partial\Omega(t)} \xi(\gamma)\, dS \right) dt \tag{15}$$

with all relevant terms as defined above.

Then minimizers (if they exist) of the energy functional E must satisfy

$$\begin{cases} \rho(\partial_t u + u \cdot \nabla u) + \nabla p = -\nabla\varphi & \text{on } \Omega(t) \\ \mathbf{div}\ u = 0 & \text{on } \Omega(t) \\ \gamma(\partial_t u_s + u_s \cdot \nabla u_s) - p\nu = \nabla_{\Sigma(t)}\sigma + H\nu\sigma & \text{on } \partial\Omega(t) \\ \partial_t \gamma + \nabla\gamma \cdot u + \gamma \mathbf{div}_{\Sigma(t)} u = 0 & \text{on } \partial\Omega(t) \end{cases} \tag{16}$$

where u_s is the Eulerian velocity of the surfactants (defined via $u_s(\eta(\beta(x,t),t),t) = \partial_t(\eta(\beta(x,t),t))$), $\sigma = \xi(\gamma) - \xi'(\gamma)\gamma$ is the surface tension, and $u, \overline{\rho}, \rho$, and p are as before.

Note that while this result and the previous result appear to be very similar, the surfactant velocity u_s is now generated not only by the motion of η but also by the motion of the surfactants β, which complicates the corresponding terms.

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