Surfactant Dynamics From The Arnold Perspective

Ethan Lu,
Carolyn Lee

Joint work with Yuxuan Liu, Jonathan Jenkins and Desmond Reed

Carnegie Mellon University

October 30, 2021

Motivation and Setup

Background

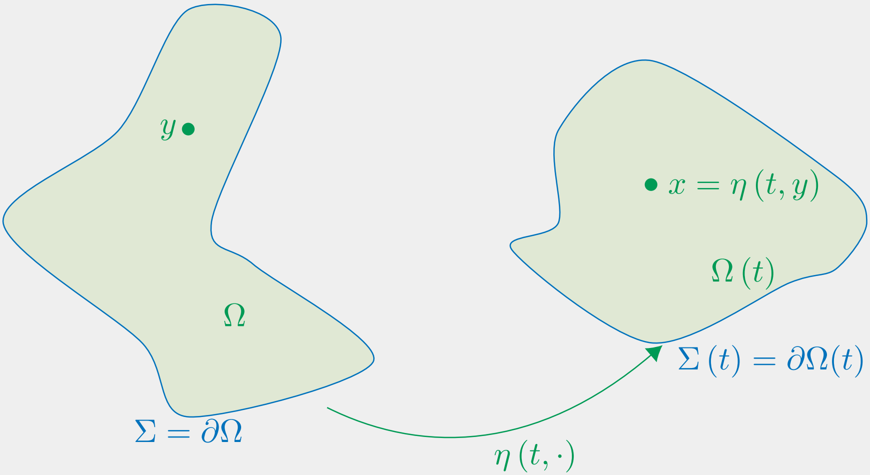
- Basic idea: analyze PDEs through **the calculus of variations**.
- Why?
  - PDEs are hard to solve!
  - Techniques including energy estimates, bootstrapping, functional analysis, etc. are often needed to do anything useful.
  - Alternative characterizations can provide other insights.
- (Arnold ’66): critical points of a particular energy are solutions to the **Euler equations**.

Background (cont)

- Next question: can the same be extended to other PDEs?
- Answer: yes!
- In particular, we're interested in those related to **surfactants**.
  - Notable examples: detergents, emulsifiers, and soap bubbles.
  - Relevant to fields like the cosmetic industry, ore extraction and in biology.

Let $\Omega \subseteq \mathbb{R}^n$ be bounded, connected and open, and set $\Sigma := \partial\Omega$ to be it's boundary and $\nu : \Sigma \to \mathbb{R}^n$ to be the associated outward pointing unit normal.
We define the function spaces $\mathrm{Diff}_0(\Omega), \mathrm{FDiff}(\Omega) \subseteq L^2(\Omega; \mathbb{R}^n)$, to be the sets of volume/orientation preserving diffeomorphisms

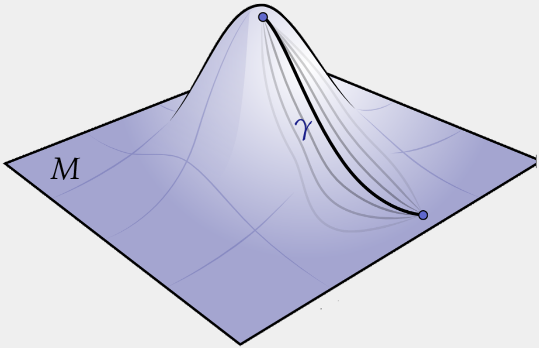
$$\mathrm{FDiff}(\Omega) = \{\eta : \Omega \to \mathbb{R}^n \mid \eta \text{ a diffeomorphism}\}.$$
$$\mathrm{Diff}_0(\Omega) = \{\eta \in \mathrm{FDiff}(\Omega) \mid \eta(\Omega) = \Omega\}.$$


y
Ω
$\Sigma = \partial\Omega$
$x = \eta(t, y)$
$\Omega(t)$
$\Sigma(t) = \partial\Omega(t)$
$\eta(t, \cdot)$

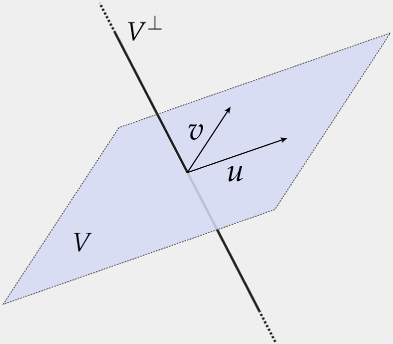
Technical Results

Key tools:

Characterizations of Perturbations



Orthogonality Conditions.



Tools from differential geometry tell us that

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

which gives us a necessary condition for locally generating a perturbation. Using techniques from ODE, we can also show that this condition is sufficient.

Let X be the space 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.

Lemma 1

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

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

Now we state 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:

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

$$H^\perp = \{\nabla p \in L^2(\Omega; \mathbb{R}^n) \mid p \in H^1(\Omega)\} \tag{5}$$

Results

Theorem 2 (Arnold)

If they exist, critical points of the energy functional $E : X \to \mathbb{R}^+$ *defined via*

$$E(\eta) = \int_0^1 \int_\Omega \frac{1}{2} |\partial_t \eta|^2 \, dxdt \tag{6}$$

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

$$\begin{cases} \partial_t u + u \cdot \nabla u + \nabla p = 0 & \text{on } \Omega \\ \textbf{div } u = 0 & \text{on } \Omega \\ u \cdot \nu = 0 & \text{on } \partial\Omega \end{cases} \tag{7}$$

where $u(\eta(x,t),t) = \partial_t \eta(x,t)$ *and* p *is the pressure.*

Proof Sketch.

- For any perturbation ζ as before, we know that we must have

$$\partial_s E(\zeta) \mid_{s=0} = 0$$

  since $\zeta(0) = \eta$ is a critical point.

- We calculate to find that $\partial_t u + u \cdot \nabla u$ must vanish when tested against any smooth, compactly supported, and divergence free function; that is

$$\partial_t u + u \cdot \nabla u \in \mathcal{V}^{\perp}$$

  (Recall: $\mathcal{V} = \{\varphi \in C_c^{\infty}(\Omega; \mathbb{R}^n) \mid \textbf{div}\ \varphi = 0\}$)

- Using the Leray decomposition, we see that this term must be exactly the negative pressure gradient, which leads to the equality

$$\partial_t u + u \cdot \nabla u + \nabla p = 0 \text{ on } \Omega.$$

$\square$

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 density 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 3

Given $\sigma \in \mathbb{R}^+$, $\overline{\rho} : \Omega \to \mathbb{R}^+$ and $\varphi \in C^1(\mathbb{R}^n)$, critical points (if they exist) of the action $A : X \to \mathbb{R}$ defined via

$$A(\eta) = \int_0^1 \left(\int_\Omega \frac{\overline{\rho}}{2} |\partial_t \eta|^2 - \varphi(\eta)\, dx - \int_{\partial\Omega(t)} \sigma dS \right) dt \tag{8}$$

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

$$\begin{cases} \rho(\partial_t u + u \cdot \nabla u) + \nabla p = -\nabla \varphi & \text{on } \Omega(t) \\ \textbf{div}\, u = 0 & \text{on } \Omega(t) \\ p = -\sigma H & \text{on } \partial\Omega(t) \end{cases} \tag{9}$$

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 $H = -\textbf{div}\, \nu$ is the mean curvature of $\partial\Omega(t)$.

Conservation of Mass

Note: We require the density ρ to satisfy the conservation of mass law:

$$\frac{d}{dt}\int_{\eta(U,t)} \rho \, dS = 0$$

for any $U \subseteq \Omega$.

Combining this with the transport equation yields

$$\partial_t \rho + \mathbf{div}(\rho u) = 0 \text{ on } \Omega(t).$$

Proof of Theorem (Sketch).

- First, we localize: by 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.

$\square$

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 4

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 $A : X \to \mathbb{R}$ via

$$A(\eta) = \int_0^1 \left(\int_\Omega \frac{\overline{\rho}}{2} |\partial_t \eta|^2 - \varphi(\eta)\, dx + \int_{\partial\Omega} \frac{\overline{\gamma}_0}{2} |\partial_t \eta|^2\, dS - \int_{\partial\Omega(t)} \xi(\gamma)\, dS \right) dt. \tag{10}$$

Then critical points (if they exist) of the action functional A must satisfy

$$\begin{cases} \rho(\partial_t u + u \cdot \nabla u) + \nabla p = -\nabla\varphi & \text{on } \Omega(t) \\ \mathbf{div}\, u = 0 & \text{on } \Omega(t) \\ \partial_t \rho + \mathbf{div}(\rho u) = 0 & \text{on } \Omega(t) \\ \gamma(\partial_t u + u \cdot \nabla u) - p\nu = \nabla_{\Sigma(t)}\sigma + H\nu\sigma & \text{on } \partial\Omega(t) \\ \partial_t \gamma + \nabla\gamma \cdot u + \gamma\, \mathbf{div}_{\Sigma(t)} u = 0 & \text{on } \partial\Omega(t) \end{cases} \tag{11}$$

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

THANKS!

- Thanks for listening!
- We'd like to thank Ian Tice, our advisor, for his guidance and mentorship throughout this project. This project was supported by funding from the NSF CAREER grant (#1653161).
- Thanks also to the organizers and Duke for hosting NCM21.
- Any questions?

References

V. I. Arnold.
On the differential geometry of infinite-dimensional Lie groups and its application to the hydrodynamics of perfect fluids.
In G. A. et al, editor, *Vladimir I. Arnold - Collected Works, vol 2.*, pages 33–69. Springer, 1966.

D. G. Ebin and J. Marsden.
Groups of diffeomorphisms and the motion of an incompressible fluid.
Annals of Mathematics, 92(1):102–163, 1970.

J. Jenkins, C. Lee, Y. Liu, E. Lu, and D. Reed.
Surfactant dynamics from the Arnold perspective.
SIAM Undergraduate Research Online(SIURO), 14, 2021.

J. Shatah and C. Zeng.
Geometry and a priori estimates for free boundary problems of the Euler equation.
Comm. Pure Appl. Math., Vol. LXI:698–744, 2007.