Control of free boundaries

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Bernoulli problem

Free boundary problem

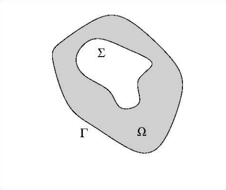
We define the set of admissible shapes as

$$\mathcal{O}_{ad} = \{\Omega \subset \mathbb{R}^2 \text{ a bounded domain : } \overline{\omega} \subset \Omega,\ \overline{\Omega} \subset \mathcal{E}\}.$$

For given $\mu \in \mathbb{R}, \mu < 0$, we consider the following free boundary problem:

$$(\mathcal{F}_\omega) : \text{Find } \Omega \in \mathcal{O}_{ad} \text{ such that}$$

$$\begin{array}{rcll} -\Delta u & = & 0 & \text{in} \quad \Omega \setminus \overline{\omega}, \\ u & = & 1 & \text{on} \quad \Sigma := \partial\omega, \\ u & = & 0 & \text{on} \quad \Gamma := \partial\Omega, \\ \partial_n u & = & \mu & \text{on} \quad \Gamma, \end{array}$$



ω is a parameter and Γ is the free boundary

Existence of solutions and control problem

- $\Omega^*(\omega)$ denotes the solution to $(\mathcal{F}_\omega)$.
- Set of admissible domains:

$$\mathcal{U}_{ad} := \{\omega \subset \mathbb{R}^2 \mid \omega_{min} \subset \omega \subset \omega_{max} \subset \mathcal{E},\ \omega \text{ is star-like with respect to all points in the ball } B_\delta(0) \text{ and } \omega \text{ is of class } \mathcal{C}^{2,\alpha}\},$$

- $\mathcal{U}_{ad}$ guarantees existence, uniqueness as well as stability of the solution to $(\mathcal{F}_\omega)$ with respect to ω [Acker, Meyer 95].
- If $\omega \in \mathcal{U}_{ad}$, then $\Omega^*(\omega)$ is of class $\mathcal{C}^\infty$ and is star-like with respect to all points in $B_\delta(0)$.
- With these assumptions there exists a unique $\Omega^*(\omega)$ solution of $(\mathcal{F}_\omega)$. We write $\Gamma^*(\omega) := \partial\Omega^*(\omega)$.
- Control problem: Find ω such that $\Gamma^*(\omega)$ is as close as possible to the boundary ∂E of a Lipschitz domain $E \in \mathcal{O}_{ad}$ such that $\omega \subset E$.

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Control of free boundaries

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Shape functionals

- We study the minimization of two functionals.
- The first functional is the measure of the symmetric difference:

$$J_1(\Omega) := |\Omega \cap E^c| + |E \cap \Omega^c| = \int_{\Omega\cap E^c} 1 \; dx + \int_{E\cap\Omega^c} 1 \; dx.$$

- $|\Omega \cap E^c| = 0$ forces Ω to be included in E.
- $|E \cap \Omega^c| = 0$ forces Ω to contain E.

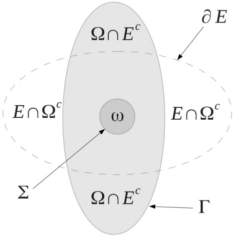


Figure : “Free” set Ω and target E

Shape functionals

- The second, "smoother", functional

$$J_2(\Omega,\omega) = \frac{1}{2}\int_{\Omega\cap E^c} u(\Omega,\omega)^2\ dx + \frac{1}{2}\int_{E\cap\omega^c} (u(\Omega,\omega) - u_l(\omega))^2\ dx,$$

where $u = u(\Omega,\omega) \in H_0^1(\mathcal{E})$ is the extension by zero to $\mathcal{E}$ of

$$\begin{aligned} -\Delta u = 0 \quad &\text{in} \quad \Omega\setminus\overline{\omega}, \\ u = 1 \quad &\text{on} \quad \Sigma := \partial\omega, \qquad u = 0 \quad \text{on} \quad \Gamma := \partial\Omega. \end{aligned}$$

The function $u_l = u_l(\omega)$ solves

$$\begin{aligned} -\Delta u_l = 0 \quad &\text{in } E\setminus\overline{\omega}, \\ u_l = 1 \quad &\text{on } \Sigma, \qquad u_l = 0 \quad \text{on } \partial E. \end{aligned}$$

Proposition

Let ω be a given open bounded set with $\omega \subset \Omega$. We have $J_1(\Omega) = 0$ and $J_2(\Omega,\omega) = 0$ if and only if $\Omega = E$ almost everywhere.

Shape optimization problem

- Bilevel shape optimization problem

$$(\mathcal{B}_i) : \begin{cases} \text{minimize} & J_i(\Omega,\omega) \\ \text{subject to} & \omega \in \mathcal{U}_{ad} \text{ and } \Omega \text{ solves } (\mathcal{F}_\omega). \end{cases}$$

The problem of minimizing $J_i(\Omega,\omega)$ over $\omega \in \mathcal{U}_{ad}$ is called the *upper-level problem*, while $(\mathcal{F}_\omega)$ is the *lower-level problem*.

- Defining the reduced functionals

$$K_1(\omega) := J_1(\Omega^*(\omega)), \qquad K_2(\omega) := J_2(\Omega^*(\omega),\omega),$$

we can rewrite the bilevel problem as

$$(\mathcal{B}_i) : \begin{cases} \text{minimize} & K_i(\omega) \\ \text{subject to} & \omega \in \mathcal{U}_{ad}. \end{cases}$$

- The minimum of $K_i(\omega)$ need not exist and need not be 0 in general. In these cases we have $\Omega^*(\omega) \neq E$ even if ω minimizes $K_i(\omega)$.

Shape derivative

- We consider perturbations of identity $I + \mathbf{V}$ where $\mathbf{V}$ is in a neighborhood of 0 in $\mathcal{C}_b^{k,\alpha}(\mathbb{R}^2, \mathbb{R}^2)$ with $k \geq 1$ and $0 < \alpha < 1$, so that $I + \mathbf{V}$ is a bi-Lipschitz homeomorphism.
- Let $T(\mathbf{V}) = I + \mathbf{V}$, $\mathbf{V} \in \mathcal{C}_b^{k,\alpha}(\mathbb{R}^2, \mathbb{R}^2)$, and denote

$$\omega_{\mathbf{V}} = T(\mathbf{V})(\omega).$$

- The functional $K(\omega)$ is Fréchet-differentiable at $\omega \subset \mathbb{R}^2$ if there exists a linear and continuous functional $\nabla K(\omega)$ from $\mathcal{C}_b^{k,\alpha}(\mathbb{R}^2, \mathbb{R}^2)$ to $\mathbb{R}$ called *shape gradient* such that

$$K(\omega_{\mathbf{V}}) = K(\omega) + \nabla K(\omega) \cdot \mathbf{V} + r(\mathbf{V}),$$

  where $|r(\mathbf{V})|/\|\mathbf{V}\|_{k,\alpha} \to 0$ as $\|\mathbf{V}\|_{k,\alpha} \to 0$.
- Define the *shape derivative* as

$$dK(\omega; \mathbf{V}) := \nabla K(\omega) \cdot \mathbf{V}.$$

Sensitivity analysis of the PDE

- Compute the shape derivative with respect to ω.
- Assume there exists $\mathbf{W}^* = \mathbf{W}^*(\mathbf{V}) \in \mathcal{C}_b^{k,\alpha}(\mathbb{R}^2, \mathbb{R}^2)$ such that

$$\Omega^*(\omega_{\mathbf{V}}) = T(\mathbf{W}^*(\mathbf{V}))(\Omega^*(\omega_0))$$

  for $\mathbf{V}$ in a neighborhood of 0.
- Since $u = u(\omega_{\mathbf{V}}, \Omega^*(\omega_{\mathbf{V}}))$, formally applying the chain rule:

$$\begin{aligned} D_{\mathbf{V}}[u(\omega_{\mathbf{V}}, \Omega^*(\omega_{\mathbf{V}}))](\widehat{\mathbf{V}}) &= D_1 u(\omega_{\mathbf{V}}, \Omega^*(\omega_{\mathbf{V}}))(\widehat{\mathbf{V}}) \\ &\quad + D_2 u(\omega_{\mathbf{V}}, \Omega^*(\omega_{\mathbf{V}}))(D_{\mathbf{V}}[T(\mathbf{W}^*(\mathbf{V}))](\widehat{\mathbf{V}})) \end{aligned}$$

- For simplicity write $\widehat{\mathbf{W}}^* := D_{\mathbf{V}}[T(\mathbf{W}^*(\mathbf{V}))](\widehat{\mathbf{V}})$ and

$$u' = u'(\widehat{\mathbf{V}}, \widehat{\mathbf{W}}^*) := D_{\mathbf{V}}[u(\omega_{\mathbf{V}}, \Omega^*(\omega_{\mathbf{V}}))](\widehat{\mathbf{V}})$$

Sensitivity analysis of the PDE

- Using shape calculus we obtain

$$
\begin{aligned}
-\Delta u' &= 0 \quad \text{in} \quad \Omega^*(\omega) \setminus \overline{\omega},\\
u' &= -\partial_n u \widehat{\mathbf{V}} \cdot \mathbf{n} \quad \text{on} \quad \Sigma,\\
u' &= -\partial_n u \widehat{\mathbf{W}}^* \cdot \mathbf{n} \quad \text{on} \quad \Gamma^*(\omega),\\
\partial_n u' &= \mathrm{div}_\Gamma(\nabla_\Gamma u \widehat{\mathbf{W}}^* \cdot \mathbf{n}) + \mu \mathcal{H} \widehat{\mathbf{W}}^* \cdot \mathbf{n} \quad \text{on} \quad \Gamma^*(\omega),
\end{aligned}
$$

- Since $\nabla_\Gamma u = 0$ and $\partial_n u = \mu$ on Γ we get

$$
\begin{aligned}
-\Delta u' &= 0 \quad \text{in} \quad \Omega^*(\omega) \setminus \overline{\omega},\\
u' &= -\partial_n u \widehat{\mathbf{V}} \cdot \mathbf{n} \quad \text{on} \quad \Sigma,\\
u' &= -\mu \widehat{\mathbf{W}}^* \cdot \mathbf{n} \quad \text{on} \quad \Gamma^*(\omega),\\
\partial_n u' &= \mu \mathcal{H} \widehat{\mathbf{W}}^* \cdot \mathbf{n} \quad \text{on} \quad \Gamma^*(\omega).
\end{aligned}
$$

Sensitivity analysis of the PDE

- Gathering the two last boundary conditions we can eliminate $\widehat{\mathbf{W}}^*$:

$$\begin{aligned} -\Delta u' = 0 \quad &\text{in} \quad \Omega^*(\omega)\setminus\overline{\omega}, \\ u' = -\partial_n u \widehat{\mathbf{V}}\cdot\mathbf{n} \quad &\text{on} \quad \Sigma, \\ \partial_n u' + \mathcal{H}u' = 0 \quad &\text{on} \quad \Gamma^*(\omega). \end{aligned}$$

  Assuming $\mathcal{H}\geq 0$, this equation has a unique solution.
- We also obtain

$$\widehat{\mathbf{W}}^*(\widehat{\mathbf{V}}) = -\mu^{-1}u'(\widehat{\mathbf{V}})\mathbf{n} \quad \text{on } \Gamma^*(\omega)$$

- The tangential component of $\widehat{\mathbf{W}}^*$ can be chosen arbitrarily according to the Hadamard-Zolésio structure theorem and is taken equal to zero.

Sensitivity analysis

Theorem

Assume that there exist two bounded open sets Ω, ω *of class* $\mathcal{C}^{m+1,\alpha}$, $m \geq 2$, $0 < \alpha < 1$ *such that* $(\mathcal{F}_\omega)$ *is satisfied in* $\Omega \setminus \overline{\omega}$. *Assume* $\mathcal{H} \geq 0$ *on* $\Gamma = \partial\Omega$. *Then there exists an open neighborhood* $\mathcal{V}$ *of* 0 *in* $\mathcal{C}_b^{m,\alpha}(\mathbb{R}^2, \mathbb{R}^2)$ *and a function*

$$\mathcal{V} \ni \mathbf{V} \mapsto \mathbf{W}^*(\mathbf{V}) \in \mathcal{C}_b^{m,\alpha}(\mathbb{R}^2, \mathbb{R}^2)$$

of class $\mathcal{C}^\infty$ *such that* $(\mathcal{F}_\omega)$ *has a solution in* $\Omega_{\mathbf{W}^*(\mathbf{V})} \setminus \overline{\omega_{\mathbf{V}}}$ *for all* $\mathbf{V} \in \mathcal{V}$ *and* $\mathbf{W}^*(0) \equiv 0$.

Main idea of the proof: Apply the implicit function theorem at $(v_n, w_n) = (0, 0)$ for the function

$$\begin{aligned} F : \mathcal{C}^{m,\alpha}(\Sigma) \times \mathcal{C}^{m,\alpha}(\Gamma) &\to \mathcal{C}^{m,\alpha}(\overline{\Omega} \setminus \omega), \\ (v_n, w_n) &\mapsto (u_{1,\mathbf{V},\mathbf{W}} - u_{2,\mathbf{V},\mathbf{W}}) \circ (I + \mathbf{V} + \mathbf{W}), \end{aligned}$$

where $\mathbf{V}|_\Sigma := v_n \mathbf{n}_\Sigma$ and $\mathbf{W}|_\Gamma := w_n \mathbf{n}_\Gamma$.

Sensitivity analysis

Corollary

Under the same assumptions as in Theorem 1, the derivative of $\mathbf{W}^*(\mathbf{V})$ *in direction* $\widehat{\mathbf{V}}$ *at* $\mathbf{V} = 0$ *in* $\mathcal{C}_b^{m,\alpha}(\mathbb{R}^2, \mathbb{R}^2)$ *is such that*

$$D_{\mathbf{V}}\mathbf{W}^*(0; \widehat{\mathbf{V}}) = -\mu^{-1}\bar{u}(\widehat{\mathbf{V}})\mathbf{n}_\Gamma \text{ on } \Gamma^*(\omega),$$

where $\bar{u}(\widehat{\mathbf{V}})$ *solves*

$$\begin{aligned} -\Delta\bar{u}(\widehat{\mathbf{V}}) &= 0 \quad \text{in} \quad \Omega^*(\omega) \setminus \overline{\omega}, \\ \bar{u}(\widehat{\mathbf{V}}) &= -\partial_n u \widehat{\mathbf{V}} \cdot \mathbf{n}_\Sigma \quad \text{on} \quad \Sigma, \\ \partial_n \bar{u}(\widehat{\mathbf{V}}) + \mathcal{H}\bar{u}(\widehat{\mathbf{V}}) &= 0 \quad \text{on} \quad \Gamma^*(\omega), \end{aligned}$$

Monotonicity

Theorem (Monotonicity)

Let Ω and ω satisfy the assumptions of Theorem 1 and let $\widehat{\mathbf{V}} \in \mathcal{C}_b^{m,\alpha}(\mathbb{R}^2, \mathbb{R}^2)$, $m \geq 2$. Assume $\mu < 0$, $\widehat{\mathbf{V}}(x) \cdot \mathbf{n}(x) \leq 0$ for all $x \in \Sigma$ and there exists $x \in \Sigma$ such that $\widehat{\mathbf{V}}(x) \cdot \mathbf{n}(x) < 0$, then $\widehat{\mathbf{W}}^*(x) \cdot \mathbf{n}(x) > 0$ for all $x \in \Gamma$.

Remark

The convexity of Ω holds whenever ω is convex.

Remark

Under the assumptions of Theorem 1 this leads to the monotonicity for the set inclusion of $\Omega^*(\omega)$ with respect to a convex ω for small perturbations of ω.

Shape derivative of K_1

Theorem

Let $\omega \subset \mathbb{R}^2$ be a bounded domain, with a boundary of class $\mathcal{C}^{2,\alpha}$, and let $\mathbf{V} \in \mathcal{C}_b^{2,\alpha}(\mathbb{R}^2, \mathbb{R}^2)$ be given. Assume $\mathcal{H} \geq 0$ on $\Gamma^*(\omega)$. Then the shape gradient $\nabla K_1(\omega)$ of the cost K_1 can be expressed as

$$\nabla K_1(\omega) = \nabla p \cdot \nabla u \in \mathcal{C}^{1,\alpha}(\Sigma),$$

where all expressions are evaluated on Σ, and the adjoint state p satisfies

$$\begin{aligned} -\Delta p &= 0 \quad \text{in} \quad \Omega^*(\omega) \setminus \overline{\omega}, \\ p &= 0 \quad \text{on} \quad \Sigma, \\ \partial_n p + \mathcal{H} p &= -\mu^{-1} \mathbb{1}_{E^c} + \mu^{-1} \mathbb{1}_E \quad \text{on} \quad \Gamma^*(\omega). \end{aligned}$$

Proof (shape derivative of K_1)

For an arbitrary $\mathbf{W} \in \mathcal{C}_b^{2,\alpha}(\mathbb{R}^2, \mathbb{R}^2)$:

$$dJ_1(\Omega; \mathbf{W}) = \int_{\Gamma \cap E^c} \mathbf{W} \cdot \mathbf{n} \, ds + \int_{\Gamma \cap E} -\mathbf{W} \cdot \mathbf{n} \, ds.$$

Since $K_1(\omega_{\mathbf{V}}) = J_1((I + \mathbf{W}^*(\mathbf{V}))(\Omega^*(\omega)))$ we may apply the chain rule

$$\begin{aligned} dK_1(\omega; \widehat{\mathbf{V}}) &= dJ_1(\Omega^*(\omega); D_{\mathbf{V}}\mathbf{W}^*(0; \widehat{\mathbf{V}})) \\ &= \int_{\Gamma^* \cap E^c} -\mu^{-1} u' \, ds + \int_{\Gamma^* \cap E} \mu^{-1} u' \, ds \\ &= \int_{\Gamma^*} (-\mu^{-1} \mathbb{1}_{E^c} + \mu^{-1} \mathbb{1}_E) u' \, ds. \end{aligned}$$

Using the adjoint state p and Green's formula in $\Omega^*(\omega) \setminus \overline{\omega}$ we obtain

$$dK_1(\omega; \widehat{\mathbf{V}}) = \int_{\Sigma} \nabla p \cdot \nabla u \; \widehat{\mathbf{V}} \cdot \mathbf{n} \, ds$$

Shape derivative for K_2

Theorem

Let $\omega \subset \mathbb{R}^2$ be a bounded domain, with a boundary of class $\mathcal{C}^{2,\alpha}$, and let $\mathbf{V} \in \mathcal{C}_b^{2,\alpha}(\mathbb{R}^2, \mathbb{R}^2)$ be given. Assume $\mathcal{H} \geq 0$ on $\Gamma^*(\omega)$. Then

$$dK_2(\omega, \widehat{\mathbf{V}}) = \int_\Sigma [\nabla u \cdot \nabla p + \nabla p_l \cdot \nabla u_l] \widehat{\mathbf{V}} \cdot \mathbf{n} \, ds,$$

and the adjoint states p_l and p satisfy

$$\begin{aligned} -\Delta p_l &= -(u - u_l) \quad \text{in } E \setminus \overline{\omega}, \\ p_l &= 0 \quad \text{on } \Sigma, \\ p_l &= 0 \quad \text{on } \partial E, \end{aligned}$$

$$\begin{aligned} -\Delta p &= u \mathbb{1}_{\Omega^*(\omega) \cap E^c} + (u - u_l) \mathbb{1}_{E \cap \omega^c} \quad \text{in } \Omega^*(\omega) \setminus \overline{\omega}, \\ p &= 0 \quad \text{on } \Sigma, \\ \partial_n p + \mathcal{H} p &= 0 \quad \text{on } \Gamma^*(\omega), \end{aligned}$$

Algorithm

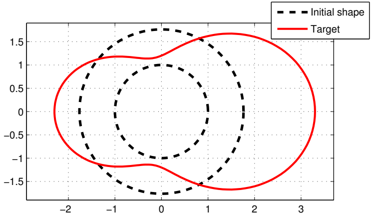
- Numerical results by Henry Kasumba.
- Solve the optimization problems using an iterative process.
- Find a solution to the free boundary problem $(\mathcal{F}_\omega)$ first.
- Then proceed to the minimization of K_1 or K_2 using a boundary variation technique.
- Use the negative shape gradients $\mathbf{V}_i = -\nabla K_i(\omega)\mathbf{n}$ on Σ as a descent direction, they need to be extended to the entire domain for the numerical method.
- Introduce an extension of $\mathbf{V}_i$ over the entire domain $\Omega^* \setminus \overline{\omega}$ such that

$$dK_i(\omega;\mathbf{V}_i) = \int_\Sigma \nabla K_i(\omega)\mathbf{V}_i\cdot\mathbf{n}\, ds = -\int_{\Omega^*\setminus\overline{\omega}} |D\mathbf{V}_i|^2 + |\mathbf{V}_i|^2\, d\mathbf{x} < 0$$

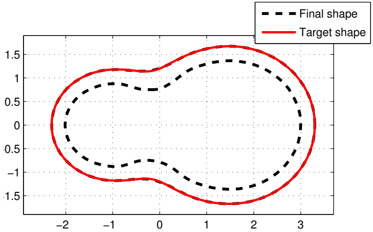
which yields a descent direction for the cost functionals $K_i,\ i = 1, 2$.

Sensitivity analysis

- Investigate the effect of increasing the value of μ while the target boundary Γ_T remains fixed.
- The initial Σ is a circle of radius 1 while Γ is a circle of radius C.
- The initial cost is $K_2(\omega^{(0)}) \approx 0.1071$.



(a) Target and initial shape

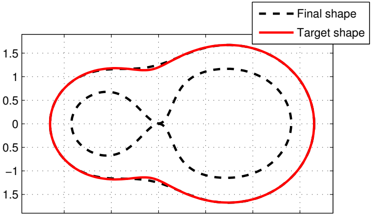


(b) Target and final shape

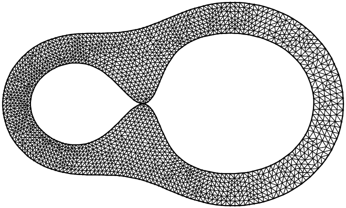
Figure : Target E, initial $\omega^{(0)}, \Omega^*(\omega^{(0)})$ and final shapes $\omega^{(final)}, \Omega^*(\omega^{(final)})$ using K_2 with $\mu = -3$. The final value of the cost K_2 after 111 optimization iterations and 7 mesh regenerations is found to be 6×10^{-5}.

Sensitivity analysis

- Next, set $\mu = -1.8$
- We choose the same initialization.
- After 120 iterations the boundary Σ intersects itself at the origin.



(a) Target and final shapes

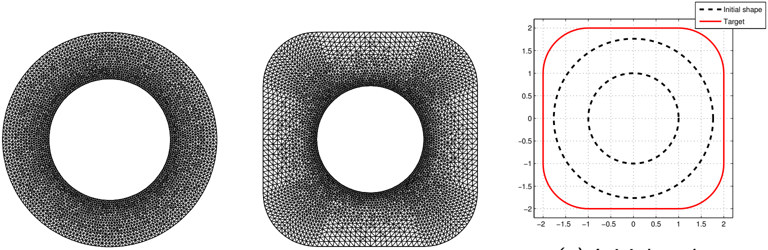


(b) Final mesh

Figure : Target shape E and final shapes $\omega^{(final)}, \Omega^*(\omega^{(final)})$ using K_2 with $\mu = -1.8$, initial value: $K_2(\omega^{(0)}) \approx 0.128$, final value: $K_2(\omega^{final}) \approx 3.28 \times 10^{-4}$.

Sensitivity analysis

- In this example we check whether there exists a domain $\omega \in \mathcal{U}_{ad}$ such that $\Gamma^*(\omega)$ is as close as possible to Γ_T not of class $\mathcal{C}^\infty$.
- We minimize K_2 with ∂E a square with rounded corners.
- The target is not of class $\mathcal{C}^\infty$. We set $\mu = -1$. Σ is initialized using a circle of radius 1 and Γ using a circle of radius C.



(a) $\Omega^*(\omega^{(0)}) \setminus \overline{\omega}^{(0)}$ *(b) Target* $E \setminus \omega^{(0)}$ *(c) Initial and target shapes*

Figure : Initial domains and target E

Sensitivity analysis

- The target Γ_T is not reached exactly. Some of the optimization variables attained the lower and upper bounds.
- The non-existence of $\omega \in \mathcal{U}_{ad}$ usually leads to oscillations of ω.
- Since we use a regularized velocity field, these oscillations of the inner boundary do not occur.

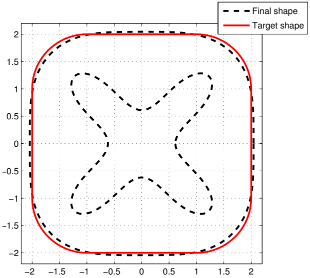
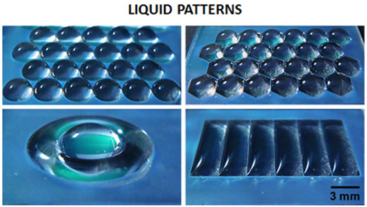


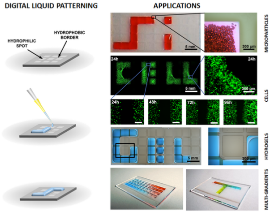
Figure : Initial and final shapes of the free boundary using K_2. Initial value : $K_2(\omega^{(0)}) \approx 0.0954102$. Final value after 20 optimization steps $K_2(\omega^{(final)}) \approx 1.1067 \times 10^{-3}$.

Summary

- The shape sensitivity analysis for the control of free boundaries can be rigorously justified for the Bernoulli problem.
- The control can be any parameter of the problem: other boundaries, boundary conditions, coefficients ...
- The existence of an induced vector field $\mathbf{W}^*$ depends on good properties of the free boundary (existence, uniqueness, regularity, continuity ...) and also on the well-posedness of the PDE for the derivative of $\mathbf{W}^*$.
- The shape derivative of the cost functional requires only the first derivative of $\mathbf{W}^*$, given by the solution of a certain PDE. In general, the well-posedness of this PDE is an issue.

Liquid And Cell Patterning





http://levkingroup.com/biofuctional-polymer-surfaces.html

Applications:

- Control the shape of sessile droplets on substrates by surface tension (lab-on-a-chip).
- Help direct the growth of biofilms and cell cultures in droplets by affecting nutrient uptake and setting desired shape.
- Affect film deposition (patterning) through droplet shape and evaporation.
- Droplet lenses.

Application References

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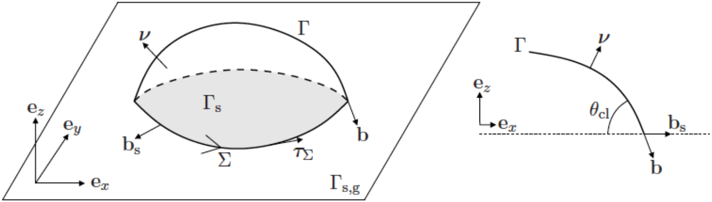
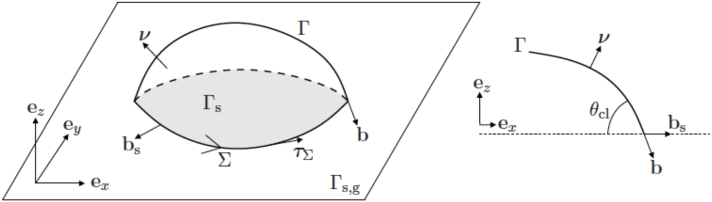
Controlling Droplet Shape



- **Goal:** Control the shape of the footprint Γ_s of a droplet by controlling the substrate surface tension.
- We are able to control the contact angle between the droplet and the substrate on the contact line Σ which is related to the "slope" of the surface Γ.

Energy of Droplets With Surface Tension



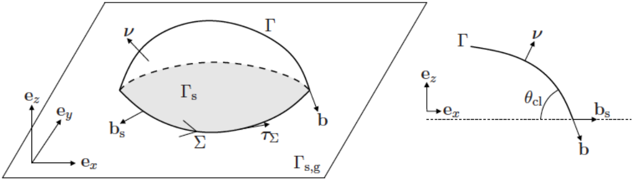
Equilibrium Model:

- Free energy of droplet Ω:

$$\mathcal{A}(\Omega) = \int_{\Gamma_s} \gamma_s + \int_{\Gamma} \gamma + \int_{\Gamma_{s,g}} \gamma_{s,g} - \int_{\Omega} G(\mathbf{x}),$$

- γ_s, γ, $\gamma_{s,g}$ are surface tension coefficients in $C^\infty(\mathcal{P})$
- $G(\mathbf{x}) := \mathbf{g} \cdot (\mathbf{x} - \mathbf{x}_0)$ where $\mathbf{g}$ = vector acceleration due to gravity.

Energy of Droplets With Surface Tension



Equilibrium Model:

- Lagrangian for the volume constraint:

$$\mathcal{L}(\Omega, p_0) = \mathcal{A}(\Omega) - p_0\left(|\Omega| - C_p\right)$$

Equilibrium

Sensitivity:

- Here the shape derivatives $\gamma_{\mathrm{s}}'(\mathbf{V}) = \gamma'(\mathbf{V}) = \gamma_{\mathrm{s,g}}'(\mathbf{V}) = G'(\mathbf{V}) \equiv 0$
- Using the shape derivative formulae:

$$D_\Omega \mathcal{L}(\Omega, p_0; \mathbf{V}) = \int_\Sigma (\gamma_{\mathrm{s}} - \gamma_{\mathrm{s,g}})\, \mathbf{b}_{\mathrm{s}} \cdot \mathbf{V} + \int_\Gamma \gamma \nabla_\Gamma \cdot \mathbf{V} - \int_\Gamma G(\mathbf{x}) \boldsymbol{\nu} \cdot \mathbf{V} - p_0 \int_\Gamma \boldsymbol{\nu} \cdot \mathbf{V},$$

  for all smooth shape perturbations $\mathbf{V}$.
- At equilibrium we have

$$D_\Omega \mathcal{L}(\Omega, p_0; \mathbf{V}) = 0 \quad \text{for all } \mathbf{V}.$$

Equilibrium

Stationarity - First Order Conditions:

- Alternatively it may be written as

$$D_\Omega \mathcal{L}(\Omega, p_0; \mathbf{V}) = \int_\Sigma (\gamma_{\mathrm{s}} - \gamma_{\mathrm{s,g}})\, \mathbf{b}_{\mathrm{s}} \cdot \mathbf{V} + \int_\Sigma \gamma\, \mathbf{b}_{\mathrm{g}} \cdot \mathbf{V} + \int_\Gamma \gamma\kappa\boldsymbol{\nu} \cdot \mathbf{V} - \int_\Gamma G(\mathbf{x})\boldsymbol{\nu} \cdot \mathbf{V} - p_0 \int_\Gamma \boldsymbol{\nu} \cdot \mathbf{V},$$

- Set $\mathbf{V} = \phi\boldsymbol{\nu}$ where $\phi : \Gamma \to \mathbb{R}$ is a smooth function with compact support on Γ.

$$\gamma\kappa - G - p_0 = 0, \quad \text{on } \Gamma, \quad \kappa = \text{total curvature of } \Gamma,$$

- Set $\mathbf{V} = \phi\mathbf{b}_{\mathrm{s}}$ near Σ with ϕ smooth and $\cos\theta_{\mathrm{cl}} = \mathbf{b}_{\mathrm{g}} \cdot \mathbf{b}_{\mathrm{s}}$.

$$\gamma\cos\theta_{\mathrm{cl}} + \gamma_{\mathrm{s}} - \gamma_{\mathrm{s,g}} = 0, \quad \text{on } \Sigma, \quad \theta_{\mathrm{cl}} = \text{contact angle of } \Gamma.$$

"Forward" Problem

Surface Tension Control:

- Let $u = \gamma_{\mathrm{s}} - \gamma_{\mathrm{s,g}} \in C^{\infty}(\mathcal{P})$ be the *control* variable.
- Set $\gamma = 1$ for simplicity.

Time March To Equilibrium:

- L^2-**gradient flow**: at each "time-step," Find $\mathbf{V}^{n+1}$, $\mathbf{X}^{n+1}$ (at time t_{n+1}) in $\mathbb{V}^n(\Gamma)$, p_0 in $\mathbb{R}$, such that

$$\int_{\Gamma} (\mathbf{V}^{n+1} \cdot \boldsymbol{\nu})(\mathbf{Y} \cdot \boldsymbol{\nu}) = -D_{\Omega}\mathcal{L}(\Omega, p_0; \mathbf{Y}) \quad \forall \mathbf{Y} \text{ in } \mathbb{V}^n(\Gamma),$$

$$\mathbf{X}^{n+1} = \mathbf{X}^n + \delta t \mathbf{V}^{n+1}, \qquad \int_{\Gamma} \mathbf{V}^{n+1} \cdot \boldsymbol{\nu} = 0,$$

where Γ is the current (known) domain at time t_n.

Desired Footprint

Objective Functional:

- One option:

$$J(\Gamma_s) = \frac{1}{2}\int_{\mathcal{P}} (\chi_{\{\Gamma_s\}} - \chi_d)^2,$$

where χ_d is the characteristic function of the desired footprint.

Desired Footprint

Objective Functional:

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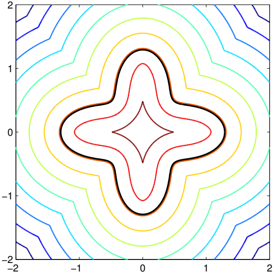


- Better option:

$$J(\Gamma_s) = \frac{1}{2}\int_{\Sigma} \phi^2, \quad \Sigma := \partial\Gamma_s \equiv \partial\Gamma.$$

- $\phi : \mathcal{P} \to \mathbb{R}$ is the distance function to Σ_d.

Reduced Functional

Optimization Problem:

- Let $\mathcal{J}(u) := J(\Gamma_{\mathrm{s}}(u))$.
- Solve this problem:

$$\begin{aligned} \text{minimize} \quad & \mathcal{J}(u) \\ \text{subject to} \quad & u \in C^\infty(\mathcal{P}), |u| \leq 1 - \varrho, \end{aligned}$$

  where $\varrho > 0$ is a small parameter
- Recall that $u = -\cos\theta_{\mathrm{cl}}$.

Shape Sensitivity

Perturbation:

- Let η be a smooth perturbation of the control:

$$u_\epsilon = u + \epsilon\eta.$$

- Parameterize the equilibrium equations:

  Find $\Omega(\epsilon)$, $\Gamma(\epsilon)$ and $p_0(\epsilon) \in \mathbb{R}$ such that

$$\int_{\Sigma(\epsilon)} [u_\epsilon \, \mathbf{b}_{\mathrm{s}}(\epsilon) + \mathbf{b}_{\mathrm{g}}(\epsilon)] \cdot \mathbf{Y} + \int_{\Gamma(\epsilon)} (\kappa(\epsilon) - G(\mathbf{x}) - p_0(\epsilon)) \boldsymbol{\nu}(\epsilon) \cdot \mathbf{Y} = 0, \quad \forall \mathbf{Y} \in \mathcal{V}$$

$$\int_{\Omega(\epsilon)} 1 = C.$$

- This *induces* a deformation of Γ, which induces a flow velocity $\mathbf{W}^* = \mathbf{W}^*(\epsilon) \in \mathcal{V}$.

Sensitivity of the free boundary Γ

Theorem

Assume there exists Γ, Σ of class C^∞ solutions of the free boundary problem for some $u \in C^\infty(\mathcal{P})$. Then there exists an open neighbourhood $\mathcal{E}$ of 0 in $\mathbb{R}$ and a function

$$\mathcal{E} \ni \epsilon \mapsto (p_0(\epsilon), \mathbf{W}^*(\epsilon)) \in \mathbb{R} \times C^\infty(\mathbb{R}^3, \mathbb{R}^3)$$

of class C^∞ such that $\Gamma_{\mathbf{W}^*(\epsilon)}$ and $\Sigma_{\mathbf{W}^*(\epsilon)}$ are solutions of the free boundary problem corresponding to $u_\epsilon = u + \epsilon\eta$ for all $\epsilon \in \mathcal{E}$ and $\mathbf{W}^*(0) = \mathbf{0}$.

Sensitivity of the free boundary Γ

Corollary

Assume there exists Γ, Σ *of class* $C^\infty(\mathcal{P})$ *solutions of the free boundary problem for some* $u \in C^\infty$. *Then the derivative of* $\mathbf{W}^*(\epsilon)$ *at* $\epsilon = 0$ *in direction* η *is given by*

$$D_\epsilon \mathbf{W}^*(0)(\eta) = A^{-1}(\eta)$$

where

$$\begin{aligned} A : C^\infty(\mathcal{P}) &\to C^\infty(\Gamma, \mathbb{R}) \\ \eta &\mapsto W_{\boldsymbol{\nu}}(\eta). \end{aligned}$$

is the solution operator corresponding to

$$-\Delta_\Gamma W_{\boldsymbol{\nu}} - (\boldsymbol{\nu} \cdot \nabla G) W_{\boldsymbol{\nu}} - q_0 = 0 \text{ on } \Gamma, \quad \text{such that } \int_\Gamma W_{\boldsymbol{\nu}} = 0,$$

$$\mathbf{b}_{\mathrm{g}} \cdot \nabla_\Gamma W_{\boldsymbol{\nu}} = -\frac{\eta}{\sin \theta_{\mathrm{cl}}} \text{ on } \Sigma.$$

Shape derivative of the cost functionals

- Consider two functionals

$$J(\Gamma_{\rm s}) = \frac{1}{2}\int_{\mathcal{P}} (\chi_{\{\Gamma_{\rm s}\}} - \chi_d)^2,$$
$$J(\Gamma_{\rm s}) = \frac{1}{2}\int_{\Sigma} \phi^2.$$

  where χ_d is the characteristic function of the desired footprint.
- $\phi : \mathcal{P} \to \mathbb{R}$ is the distance function to Σ_d.
- Reduced functionals

$$\mathcal{J}_i(u) := J_i(\Gamma_{\rm s}(u)), \quad i = 1, 2.$$

Shape derivative of the cost functionals

Theorem (Shape Derivative of $\mathcal{J}_1$)

Assume there exists Γ, Σ *of class* C^∞ *solutions of the free boundary problem for some* $u \in C^\infty(\mathcal{P})$. *Then the shape derivative of* $\mathcal{J}_1$ *is*

$$D\mathcal{J}_1(u;\eta) = -\int_\Sigma \frac{\eta}{\sin\theta_{\mathrm{cl}}} Z_{\boldsymbol{\nu}},$$

where the adjoint states $Z_{\boldsymbol{\nu}}, r_0$ *satisfy*

$$-\Delta_\Gamma Z_{\boldsymbol{\nu}} - (\boldsymbol{\nu}\cdot\nabla G) Z_{\boldsymbol{\nu}} - r_0 = 0 \text{ on } \Gamma, \quad \text{such that } \int_\Gamma Z_{\boldsymbol{\nu}} = 0,$$

$$\mathbf{b}_{\mathrm{g}} \cdot \nabla_\Gamma Z_{\boldsymbol{\nu}} = \frac{\zeta}{\sin\theta_{\mathrm{cl}}} \text{ on } \Sigma,$$

where $\zeta(x) = -1$ *in* Γ_d *and* $\zeta(x) = 1$ *in* Γ_d^c.

Shape derivative of the cost functionals

Theorem (Shape Derivative of $\mathcal{J}_2$)

Assume there exists Γ, Σ of class C^∞ solutions of the free boundary problem for some $u \in C^\infty(\mathcal{P})$. Then the shape derivative of $\mathcal{J}_2$ is

$$D\mathcal{J}_2(u;\eta) = -\int_\Sigma \frac{\eta}{\sin\theta_{\mathrm{cl}}} Z_{\boldsymbol{\nu}},$$

where the adjoint states $Z_{\boldsymbol{\nu}}, r_0$ satisfy

$$-\Delta_\Gamma Z_{\boldsymbol{\nu}} - (\boldsymbol{\nu}\cdot\nabla G)Z_{\boldsymbol{\nu}} - r_0 = 0 \text{ on } \Gamma, \quad \text{such that } \int_\Gamma Z_{\boldsymbol{\nu}} = 0,$$

$$\mathbf{b}_{\mathrm{g}}\cdot\nabla_\Gamma Z_{\boldsymbol{\nu}} = \frac{1}{2\sin\theta_{\mathrm{cl}}}[(\mathbf{b}_{\mathrm{s}}\cdot\nabla)\phi^2 + \kappa_\Sigma\phi^2] \text{ on } \Sigma.$$

Numerical results

Numerical results by Shawn W. Walker.

Videos: Ellipse Footprint, Square Footprint, Clover Footprint

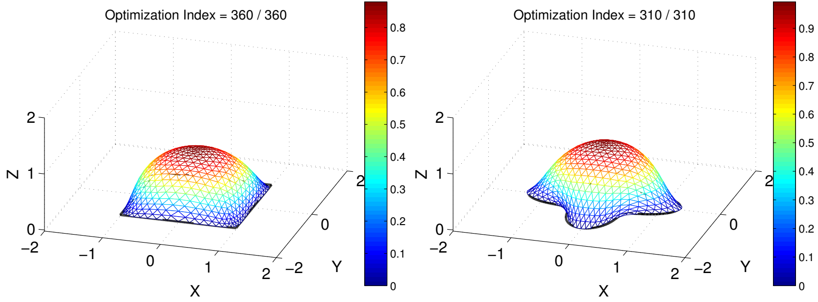


Figure : Optimal droplet shapes for the square (left) and the clover (right).

Numerical results

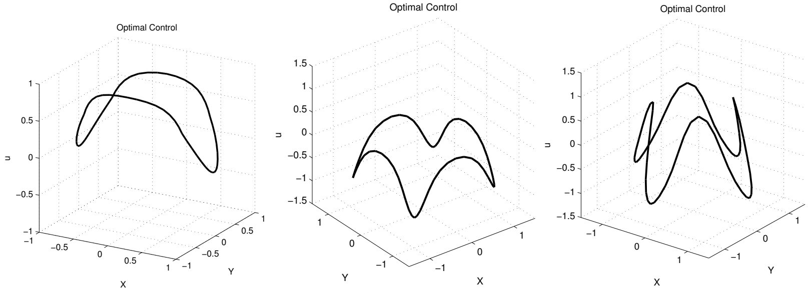
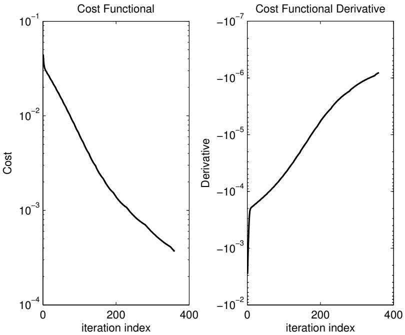


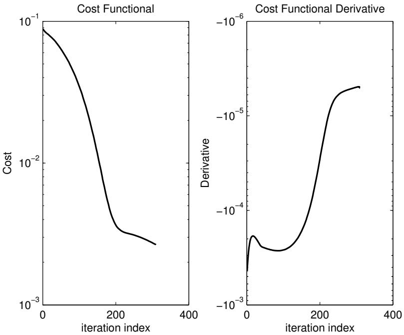
Figure : Optimal control for the ellipse (left), square (center) and clover (right).

Optimization History

Square Footprint



Clover Footprint



Muito obrigado e Feliz Aniversário Jan!