Introduction to Shape Optimization

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Frontiers in PDE-constrained Optimization

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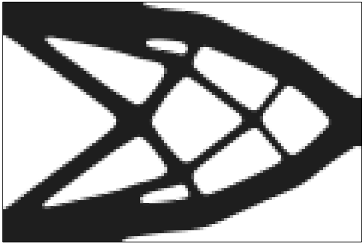
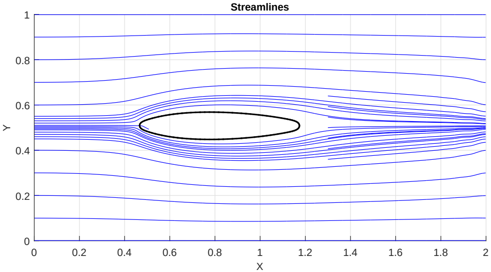
Examples of Shape Optimization

- Optimal shape of structures (G. Allaire, et al).
- Inverse problems (shape detection).
- Image processing.
- Flow control.
- Minimum drag bodies.





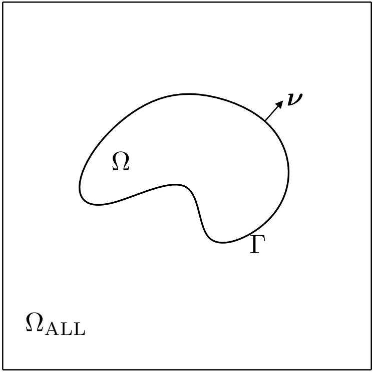
Mathematical Statement

Admissible Set:

- Let Ω_{ALL} be a "hold-all" domain.
- Optimization variable is Ω or Γ.
- Denote the admissible set by $\mathcal{U}$.
- $\mathcal{U}$ should have a *compactness* property.

Cost Functional:

- Let $\mathcal{J} : \mathcal{U} \to \mathbb{R}$ be a *shape functional*.
- Ex: $\mathcal{J}(\Omega) = \int_{\Omega} f(\mathbf{x}, \Omega)\, d\mathbf{x}$.
- Ex: $\mathcal{J}(\Gamma) = \int_{\Gamma} g(\mathbf{x}, \Gamma)\, dS(\mathbf{x})$.



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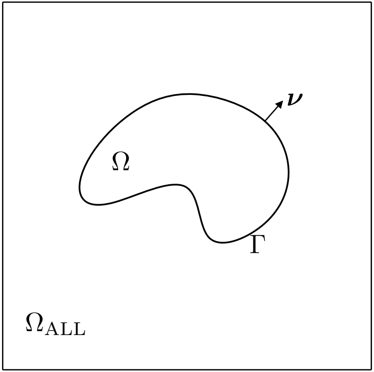
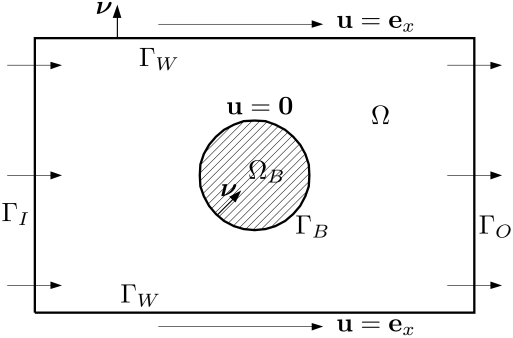


Optimization Problem:

$$\Omega^* = \arg\min_{\Omega \in \mathcal{U}} \mathcal{J}(\Omega), \qquad \Gamma^* = \arg\min_{\Gamma \in \mathcal{U}} \mathcal{J}(\Gamma).$$

Shape Optimization Example: Drag Minimization

- Define $\Omega = \Omega_{\mathrm{ALL}} \setminus \Omega_B$.



Navier-Stokes Equations:

$$
\begin{aligned}
(\mathbf{u} \cdot \nabla)\mathbf{u} - \nabla \cdot \boldsymbol{\sigma} &= \mathbf{0}, \text{ in } \Omega, \\
\nabla \cdot \mathbf{u} &= 0, \text{ in } \Omega, \\
\mathbf{u} &= \mathbf{0}, \text{ on } \Gamma_B, \\
\mathbf{u} &= \mathbf{e}_x, \text{ on } \Gamma_I, \\
\mathbf{u} &= \mathbf{e}_x, \text{ on } \Gamma_W, \\
\boldsymbol{\sigma}\boldsymbol{\nu} &= \mathbf{0}, \text{ on } \Gamma_O.
\end{aligned}
$$

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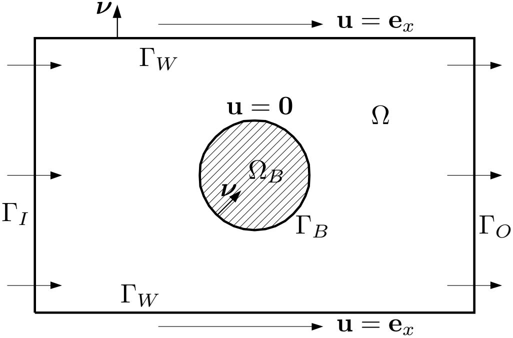
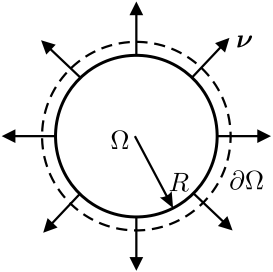


Navier-Stokes Equations:

$$\begin{aligned} (\mathbf{u} \cdot \nabla)\mathbf{u} - \nabla \cdot \boldsymbol{\sigma} &= \mathbf{0}, \text{ in } \Omega, \\ \nabla \cdot \mathbf{u} &= 0, \text{ in } \Omega, \\ \mathbf{u} &= \mathbf{0}, \text{ on } \Gamma_B, \\ \mathbf{u} &= \mathbf{e}_x, \text{ on } \Gamma_I, \\ \mathbf{u} &= \mathbf{e}_x, \text{ on } \Gamma_W, \\ \boldsymbol{\sigma}\boldsymbol{\nu} &= \mathbf{0}, \text{ on } \Gamma_O. \end{aligned}$$

- Cost functional: $\mathcal{J}(\Omega) = -\mathbf{e}_x \cdot \int_{\Gamma_B} \boldsymbol{\sigma}(\mathbf{u}, p)\boldsymbol{\nu}$ (drag force).
- Newtonian fluid: $\boldsymbol{\sigma}(\mathbf{u}, p) := -pI + \frac{2}{\text{Re}} D(\mathbf{u})$, $D(\mathbf{u}) := \frac{\nabla \mathbf{u} + (\nabla \mathbf{u})^{\dagger}}{2}$.
- Reynolds number: $\text{Re} = \frac{\rho U_0 L}{\mu}$.

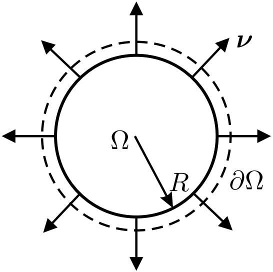
Shape Sensitivity: Simple Example



- Let Ω be a disk of radius R.
- The boundary is $\partial\Omega$ with outer normal $\boldsymbol{\nu}$.
- Let $f = f(x, y)$ be a smooth function defined everywhere.
- Suppose f also depends on Ω: $f = f(x, y; \Omega)$.
- Consider the cost functional:

$$\mathcal{J}(\Omega) = \int_{\Omega} f(x, y; \Omega)\, dx\, dy$$

Shape Sensitivity: Simple Example



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- Consider the cost functional:

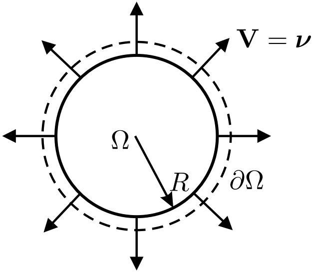
$$\mathcal{J}(\Omega) = \int_{\Omega} f(x, y; \Omega)\, dx\, dy$$

- What is the *sensitivity* of $\mathcal{J}$ with respect to changing R?
- Polar coordinates: $\mathcal{J} = \int_0^{2\pi} \int_0^R f(r, \theta; R)\, r\, dr\, d\theta$.
- Differentiate:

$$\frac{d}{dR}\mathcal{J} = \int_0^{2\pi} \left(\frac{d}{dR} \int_0^R f(r, \theta; R)\, r\, dr \right) d\theta$$

$$= \int_0^{2\pi} \int_0^R f'(r, \theta; R)\, r\, dr\, d\theta + \int_0^{2\pi} f(R, \theta; R)\, R\, d\theta.$$

Shape Sensitivity: Simple Example

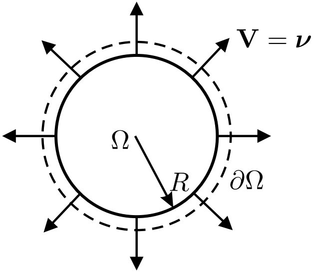


- Change back to Cartesian coordinates:

$$\frac{d}{dR}\mathcal{J} = \int_{\Omega} f'(x, y; \Omega)\, dx\, dy + \int_{\partial\Omega} f(x, y; \Omega)\, dS(x, y),$$

where f' is the derivative with respect to R.

Shape Sensitivity: Simple Example



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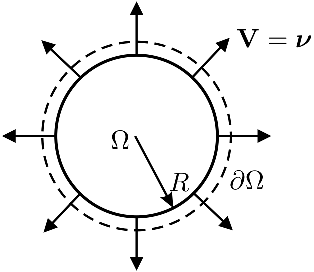
where f' is the derivative with respect to R.

- Indeed, f' is actually the derivative with respect to deforming Ω!
- Here, Ω is deformed by the "flow field" $\mathbf{V} = \boldsymbol{\nu}$.

Shape Sensitivity: Simple Example



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where f' is the derivative with respect to R.

- Indeed, f' is actually the derivative with respect to deforming Ω!
- Here, Ω is deformed by the "flow field" $\mathbf{V} = \boldsymbol{\nu}$.
- We have shown a specific version of a more general formula:

$$\delta\mathcal{J}(\Omega; \mathbf{V}) = \int_{\Omega} f'(\mathbf{x}; \Omega)\, d\mathbf{x} + \int_{\partial\Omega} f(\mathbf{x}; \Omega)\, \mathbf{V}(\mathbf{x}) \cdot \boldsymbol{\nu}(\mathbf{x})\, dS(\mathbf{x}),$$

where $\mathbf{V}$ is the instantaneous velocity deformation of Ω.

Notation!

- Vectors: e.g. $\mathbf{x} = (x, y, z)^\dagger$, $\mathbf{a} = (a_1, a_2, a_3)^\dagger$, etc., are **column** vectors.
- Gradients are **row** vectors:

$$\nabla_{\mathbf{x}} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right),$$

$$\nabla_{\mathbf{x}} = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3} \right),$$

where $\mathbf{x} = (x, y, z)^\dagger$ or $\mathbf{x} = (x_1, x_2, x_3)^\dagger$.

Notation!

- Integral notation:

$$\int_{\Omega} f(\mathbf{x})\, d\mathbf{x} = \iiint_{\Omega} f(x_1, x_2, x_3)\, dx_1\, dx_2\, dx_3,$$

- Sometimes we drop the arguments and differentials:

$$\int_{\Omega} f(\mathbf{x})\, d\mathbf{x} \equiv \int_{\Omega} f, \quad \int_{\Gamma} f(\mathbf{x})\, dS(\mathbf{x}) \equiv \int_{\Gamma} f, \quad \int_{\Sigma} f(\mathbf{x})\, d\alpha(\mathbf{x}) \equiv \int_{\Sigma} f.$$

- The measure of a set is denoted $|\cdot|$, i.e.

$$|\Omega| = \int_{\Omega} 1, \quad |\Gamma| = \int_{\Gamma} 1, \quad |\Sigma| = \int_{\Sigma} 1,$$

i.e. $|\Omega|$ is the volume of Ω, $|\Gamma|$ is the surface area of Γ, and $|\Sigma|$ is the arc-length of the curve Σ.

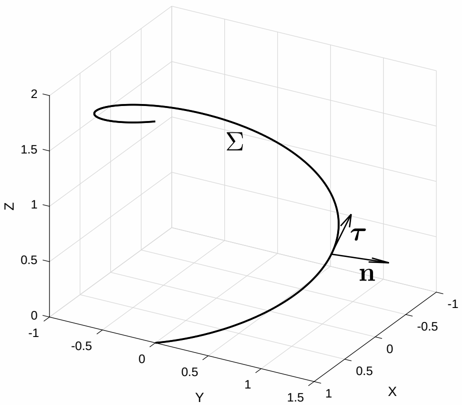
Parametric Curves

- Let $\boldsymbol{\alpha} : I \to \mathbb{R}^3$ parameterize a curve $\Sigma = \boldsymbol{\alpha}(I)$.
- Assume $|\boldsymbol{\alpha}'(t)| \neq 0$ for all $t \in I$.
- *Arc-length*:

$$\alpha(t) = \int_0^t |\boldsymbol{\alpha}'(t)| \, dt.$$

- Derivative with respect to arc-length α:

$$\frac{d}{d\alpha} = \frac{1}{|\boldsymbol{\alpha}'(t)|} \frac{d}{dt}.$$



Example: $\boldsymbol{\alpha}(t) = (\cos(2\pi t), \sin(2\pi t), 2t)^\dagger$, for all $t \in I = [0, 1]$.

Parametric Curves

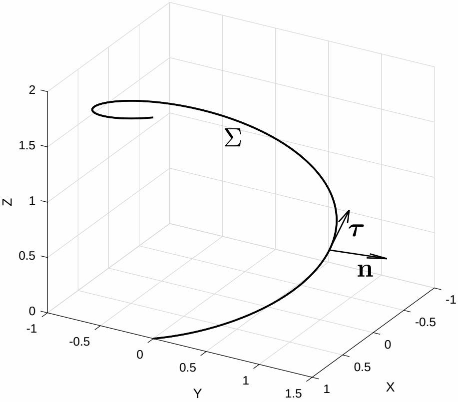
- Tangent vector:

$$\boldsymbol{\tau}(t) := \frac{\boldsymbol{\alpha}'(t)}{|\boldsymbol{\alpha}'(t)|}, \quad \text{or} \quad \boldsymbol{\tau} = \frac{d\boldsymbol{\alpha}}{d\alpha}.$$

- Curvature vector:

$$k\mathbf{n} := -\frac{d^2\boldsymbol{\alpha}}{d\alpha^2} = -\frac{d\boldsymbol{\tau}}{d\alpha},$$

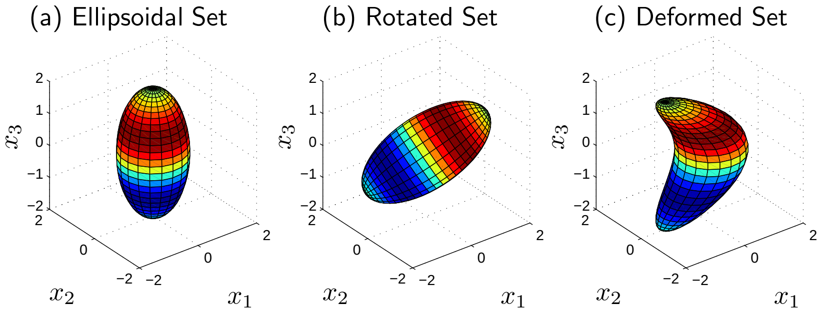
  where $\mathbf{n}$ is the unit normal vector.
- k is the *signed curvature*.



Formula in terms of t:

$$k(t)\mathbf{n}(t) = -\frac{1}{|\boldsymbol{\alpha}'(t)|}\left(\frac{\boldsymbol{\alpha}'(t)}{|\boldsymbol{\alpha}'(t)|}\right)' = -\frac{\boldsymbol{\alpha}''(t)}{\boldsymbol{\alpha}'(t)\cdot\boldsymbol{\alpha}'(t)} - \left(\frac{1}{|\boldsymbol{\alpha}'(t)|}\right)'\boldsymbol{\tau}(t)$$

Mappings



- A mapping $\mathbf{\Phi} = (\Phi_1, \Phi_2, \Phi_3)^\dagger$ can be viewed as a deformation.
- Ex: (b) rigid motion: $\mathbf{\Phi}(\mathbf{x}) = \mathbf{R}\mathbf{x} + \mathbf{b}$.
- Ex: (c) $\mathbf{\Phi}(\mathbf{x}) = (x_1 - 1.2 + 1.6\cos(x_3\pi/4), x_2, x_3)^\dagger$.

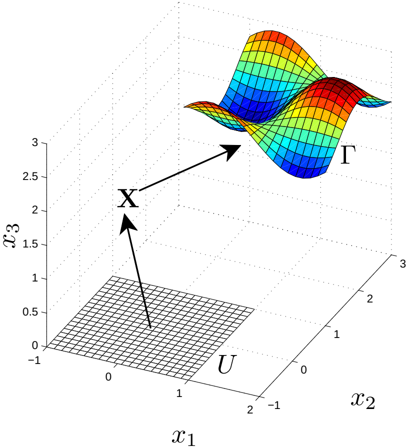
Parametric Representation of a Surface

- Think of creating a surface by deforming a flat rubber sheet into a curved sheet.
- Let $U \subset \mathbb{R}^2$ be a "flat" domain (reference domain).

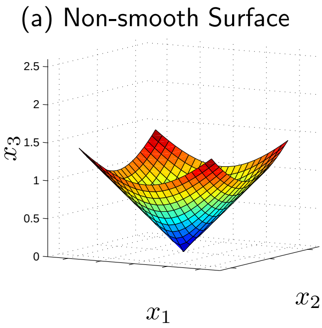
- Let $\mathbf{X} : U \to \mathbb{R}^3$ be the parameterization.
- $(s_1, s_2)^\dagger$ in U are the parameters.
- Every point $\mathbf{x} = (x_1, x_2, x_3)^\dagger$ in $\mathbb{R}^3$ is given by

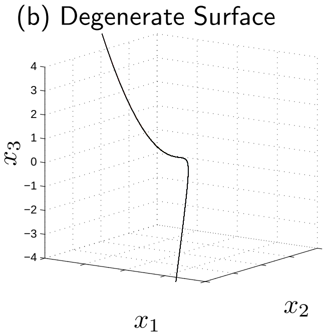
$$\mathbf{x} = \mathbf{X}(s_1, s_2).$$

- $\Gamma = \mathbf{X}(U)$ denotes the surface obtained from "deforming" U.



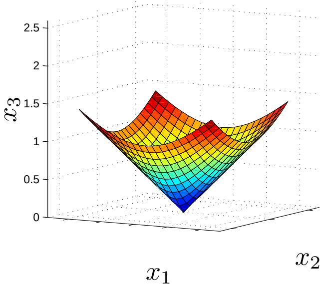
Basic Assumptions



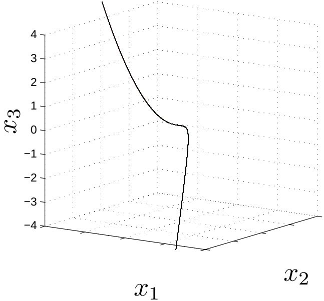


Basic Assumptions

(a) Non-smooth Surface



(b) Degenerate Surface



- Assume that $\mathbf{X}$ is smooth and injective.
- Example where $\mathbf{X}$ is **not** smooth:

$$\mathbf{X}(s_1, s_2) = \left(s_1, s_2, \sqrt{s_1^2 + s_2^2}\right)^\dagger$$

- Define the 3×2 Jacobian matrix

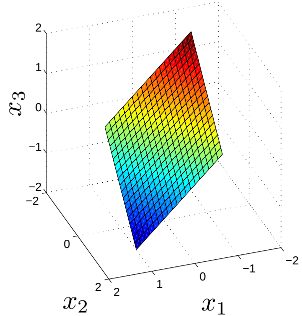
$$J = [\partial_{s_1}\mathbf{X}, \partial_{s_2}\mathbf{X}] = \nabla_{\mathbf{s}}\mathbf{X}$$

- Assume $J : U \to \mathbb{R}^{3\times 2}$ has rank 2.
- Example where this is **not** satisfied:

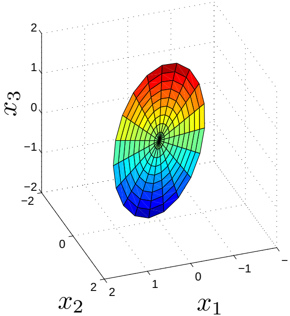
$$\mathbf{X}(s_1, s_2) = (s_1 + s_2, (s_1 + s_2)^2, (s_1 + s_2)^3)^\dagger$$

Parameterization of a Plane

(a) Cartesian parameterization



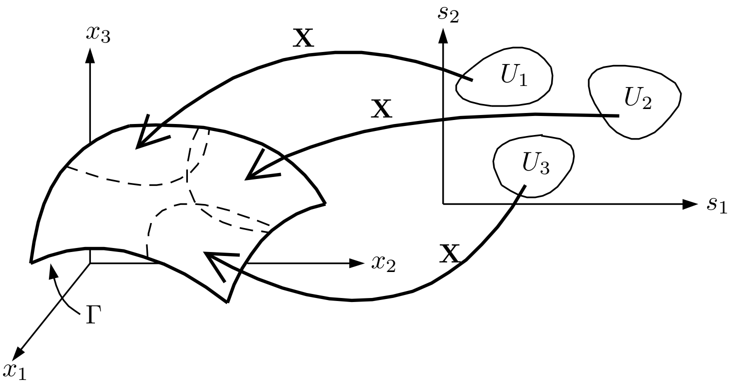
(b) Polar coordinates



- Plane: $\{\mathbf{x} \in \mathbb{R}^3 : \mathbf{x} \cdot \mathbf{N} = 0\}$, $\mathbf{N} = (N_1, N_2, N_3)^\dagger$.
  Solve for x_3: $x_3 = \frac{-1}{N_3}(x_1 N_1 + x_2 N_2)$.
- (a) $\mathbf{X}(s_1, s_2) = \left(s_1, s_2, -\frac{s_1 N_1 + s_2 N_2}{N_3}\right)^\dagger$, for all $(s_1, s_2)^\dagger$ in U, where $U = \mathbb{R}^2$.
- (b) $\mathbf{X}(r, \theta) = \left(r\cos\theta, r\sin\theta, -r\frac{\cos\theta N_1 + \sin\theta N_2}{N_3}\right)^\dagger$, where $U = (0, \infty) \times (0, 2\pi)$.

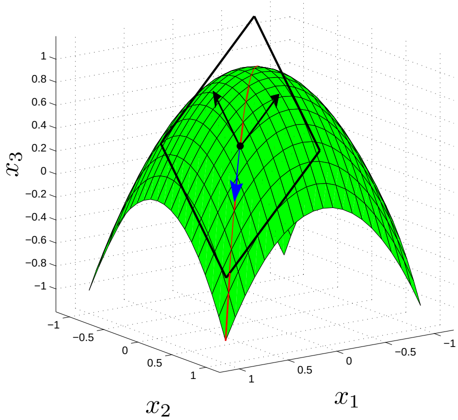
Regular Surface; Local Charts

- A **regular surface** is built from *many* maps and reference domains $(U, \mathbf{X})$.
- We call $(U, \mathbf{X})$ a **local chart**.
- For a general surface, one needs an **atlas** of local charts: $\{(U_i, \mathbf{X}_i)\}$.



Basic Properties

- The local charts $(U, \mathbf{X})$ that make up a regular surface must be sufficiently smooth.
- The surface must have a well-defined **tangent plane**.
- Tangent plane is spanned by $\{\partial_{s_1}\mathbf{X}, \partial_{s_2}\mathbf{X}\}$.



Notation:

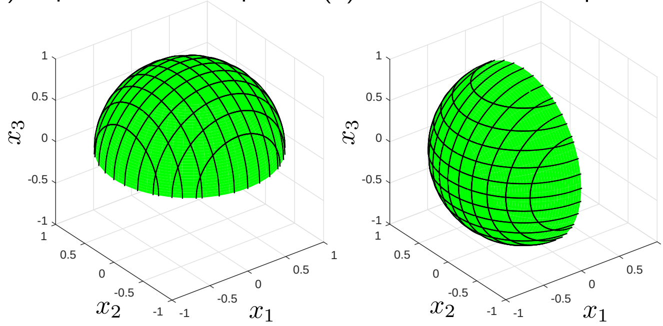
- Let $T_{\mathbf{x}}(\Gamma)$ denote the tangent plane of the surface Γ at the point $\mathbf{x}$.

First Fundamental Form

- Deforming the reference domain *distorts* it.
- Need a characterization of the distortion.
- Define the coefficients of the **First Fundamental Form**:

$$g_{ij} = \partial_{s_i} \mathbf{X} \cdot \partial_{s_j} \mathbf{X}, \quad \text{for } 1 \leq i, j \leq 2.$$

(a) Top-Half Of Unit Sphere (b) Side-Half Of Unit Sphere



Example: Plane

Recall the cartesian parameterization of a plane:

- $\mathbf{X}(s_1, s_2) = \left(s_1, s_2, -\frac{s_1 N_1 + s_2 N_2}{N_3}\right)^{\dagger}$.
- Compute: $\partial_{s_1}\mathbf{X} = \left(1, 0, -\frac{N_1}{N_3}\right)^{\dagger}, \partial_{s_2}\mathbf{X} = \left(0, 1, -\frac{N_2}{N_3}\right)^{\dagger}$.
- First fundamental form coefficients are:

$$\begin{aligned} g_{11} &= \partial_{s_1}\mathbf{X} \cdot \partial_{s_1}\mathbf{X} = 1 + (N_1/N_3)^2, \\ g_{12} &= \partial_{s_1}\mathbf{X} \cdot \partial_{s_2}\mathbf{X} = g_{21} = (N_1/N_3)(N_2/N_3), \\ g_{22} &= \partial_{s_2}\mathbf{X} \cdot \partial_{s_2}\mathbf{X} = 1 + (N_2/N_3)^2, \end{aligned}$$

which are all constant.

Example: Sphere

Consider the parameterization of part of a sphere:

- $\{(x_1, x_2, x_3)^\dagger \in \mathbb{R}^3 : x_1^2 + x_2^2 + x_3^2 = 1\}$.
- Top-half: $\mathbf{X}_1(s_1, s_2) = \left(s_1, s_2, +\sqrt{1 - (s_1^2 + s_2^2)}\right)^\dagger$, for all $(s_1, s_2)^\dagger$ in $U = \{(s_1, s_2)^\dagger \in \mathbb{R}^2 : s_1^2 + s_2^2 < 1\}$.

$$\text{Compute: } \partial_{s_1}\mathbf{X}(s_1, s_2) = \left(1, 0, -s_1(1 - (s_1^2 + s_2^2))^{-1/2}\right)^\dagger,$$

$$\partial_{s_2}\mathbf{X}(s_1, s_2) = \left(0, 1, -s_2(1 - (s_1^2 + s_2^2))^{-1/2}\right)^\dagger.$$

- First fundamental form coefficients are:

$$g_{11} = \partial_{s_1}\mathbf{X} \cdot \partial_{s_1}\mathbf{X} = \frac{1 - s_2^2}{1 - (s_1^2 + s_2^2)},$$

$$g_{12} = \partial_{s_1}\mathbf{X} \cdot \partial_{s_2}\mathbf{X} = g_{21} = \frac{s_1 s_2}{1 - (s_1^2 + s_2^2)},$$

$$g_{22} = \partial_{s_2}\mathbf{X} \cdot \partial_{s_2}\mathbf{X} = \frac{1 - s_1^2}{1 - (s_1^2 + s_2^2)},$$

which blow-up as $(s_1^2 + s_2^2) \to 1$.

Metric Tensor

- The coefficients g_{ij} can be grouped into a 2×2 matrix denoted g:

$$g = \begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix} = (\nabla_{\mathbf{s}} \mathbf{X})^{\dagger} (\nabla_{\mathbf{s}} \mathbf{X}),$$

  which is a **symmetric** matrix because $g_{12} = g_{21}$.
- g is **positive definite** for a regular surface.
- The inverse matrix:

$$g^{-1} = \begin{bmatrix} g^{11} & g^{12} \\ g^{21} & g^{22} \end{bmatrix} = \frac{1}{\det(g)} \begin{bmatrix} g_{22} & -g_{12} \\ -g_{21} & g_{11} \end{bmatrix};$$

  note the *superscript* indices.
- Of course, we have the following property because $g\, g^{-1} = I$:

$$\delta_{ij} = \sum_{k=1}^{2} g_{ik} g^{kj} = \sum_{k=1}^{2} g_{ik} g^{jk},$$

  where δ_{ij} is the "Kronecker delta":

$$\delta_{ij} = \begin{cases} 0, & \text{if } i \neq j, \\ 1, & \text{if } i = j. \end{cases}$$

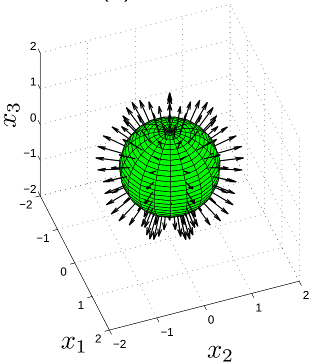
Normal Vector

- If $\mathbf{X}$ parameterizes a surface, then the **normal vector** $\boldsymbol{\nu}$ is given by

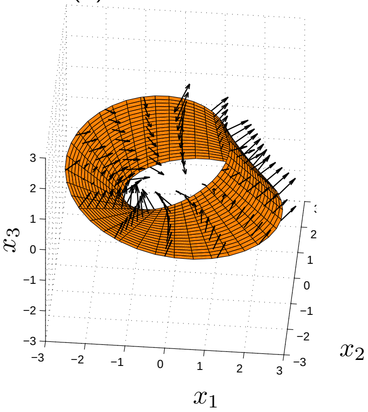
$$\boldsymbol{\nu}(\mathbf{s}) = \boldsymbol{\nu}(s_1, s_2) = \frac{\partial_{s_1}\mathbf{X}(\mathbf{s}) \times \partial_{s_2}\mathbf{X}(\mathbf{s})}{|\partial_{s_1}\mathbf{X}(\mathbf{s}) \times \partial_{s_2}\mathbf{X}(\mathbf{s})|} = \frac{\partial_{s_1}\mathbf{X}(\mathbf{s}) \times \partial_{s_2}\mathbf{X}(\mathbf{s})}{\sqrt{\det g}}$$

- Choice of parameterization induces an **orientation** of the surface.

(a) Orientable



(b) Non-orientable



Surface Area

- Let $(U, \mathbf{X})$ be a local chart of Γ, with $R = \mathbf{X}(U) \subset \Gamma$.
- The area of R is given by

$$|R| := \int_R 1 = \iint_U |\partial_{s_1}\mathbf{X} \times \partial_{s_2}\mathbf{X}| \, ds_1 \, ds_2 = \iint_U \sqrt{\det g(s_1, s_2)} \, ds_1 \, ds_2,$$

  where $g = g(s_1, s_2)$ is the metric tensor.
- Standard change of variable formula for surface integrals.

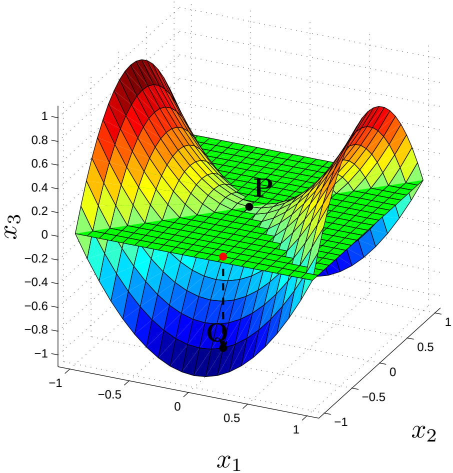
Deviating From The Tangent Plane

- Curved surface Γ.
- Tangent plane $T_P(\Gamma)$ in green.
- Let $P = \mathbf{X}(s_1, s_2)$ and $Q = \mathbf{X}(s_1 + \ell_1, s_2 + \ell_2)$.
- distance: $\operatorname{dist}(Q, T_P(\Gamma)) =$

$$\frac{1}{2} \sum_{i,j=1}^{2} \ell_i \ell_j \underbrace{\partial_{s_i} \partial_{s_j} \mathbf{X} \cdot \boldsymbol{\nu}}_{=h_{ij}}$$

$$+ \text{H.O.T.}$$

where $\boldsymbol{\nu}$ is the normal vector of Γ at P.



- h_{ij} are the coefficients of the second fundamental form.

Second Fundamental Form

Define the coefficients of the **second fundamental form**:

$$h_{ij} = \boldsymbol{\nu} \cdot \partial_{s_i} \partial_{s_j} \mathbf{X}, \text{ for } 1 \leq i, j \leq 2,$$

Since $\boldsymbol{\nu} \cdot \partial_{s_j} \mathbf{X} = 0$ for $j = 1, 2$, we can differentiate to see that

$$\partial_{s_i} \boldsymbol{\nu} \cdot \partial_{s_j} \mathbf{X} + \boldsymbol{\nu} \cdot \partial_{s_i} \partial_{s_j} \mathbf{X} = 0, \text{ for } 1 \leq i, j \leq 2.$$

Hence, we can write

$$h_{ij} = -\partial_{s_i} \boldsymbol{\nu} \cdot \partial_{s_j} \mathbf{X} = \boldsymbol{\nu} \cdot \partial_{s_i} \partial_{s_j} \mathbf{X}, \text{ for } 1 \leq i, j \leq 2.$$

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- The coefficients h_{ij} can be grouped into a 2×2 matrix denoted h:

$$h = \begin{bmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{bmatrix},$$

  which is a **symmetric** matrix because $h_{12} = h_{21}$.
- h is *not necessarily* positive definite.
- Alternative formula:

$$h = -(\nabla_{\mathbf{s}} \boldsymbol{\nu})^{\dagger} (\nabla_{\mathbf{s}} \mathbf{X}).$$

Shape Operator and Curvature

- Define the 2×2 matrix $S := -hg^{-1}$.
- This is the **shape operator** of the surface.
- The eigenvalues of S are the **principle curvatures** κ_1 and κ_2.
- κ_1 and κ_2 do *not* depend on the parameterization.

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- κ_1 and κ_2 do *not* depend on the parameterization.

Definitions of Curvature:

- Summed curvature: $\kappa := \kappa_1 + \kappa_2$.
- Vector curvature: $\boldsymbol{\kappa} := \kappa \boldsymbol{\nu}$.
- Gauss curvature: $\kappa_G := \kappa_1 \kappa_2$.

Formulas:

- Summed curvature:

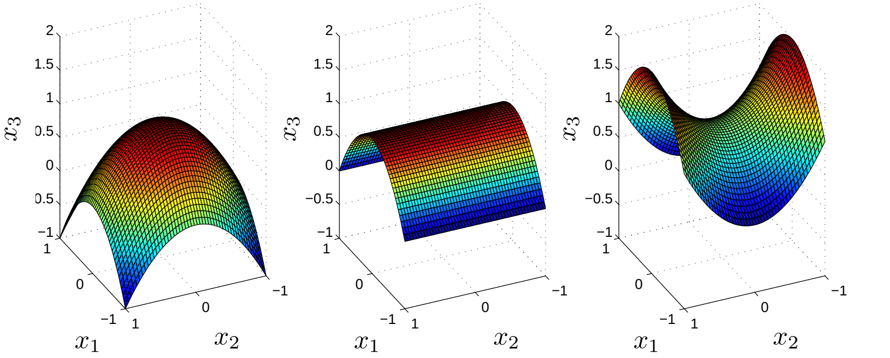
$$\kappa := \operatorname{trace} S = -\sum_{i,j=1}^{2} g^{ij} h_{ij}$$

- Gauss curvature:

$$\kappa_G := \det S = \frac{\det(-h)}{\det g} = \frac{\det h}{\det g}$$

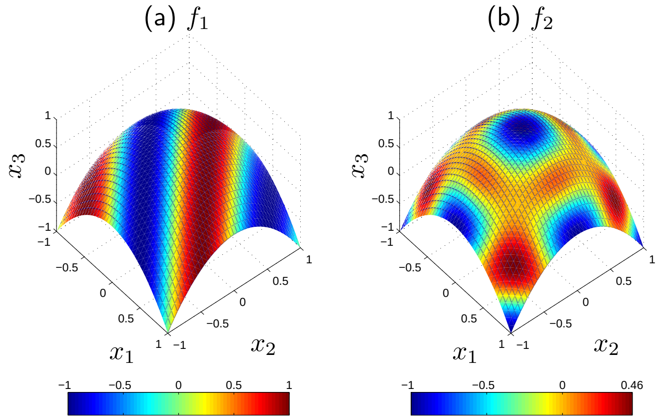
Classification of Surfaces

(a) Elliptic ($\kappa_G > 0$) (b) Parabolic ($\kappa_G = 0$) (c) Hyperbolic ($\kappa_G < 0$)



- The Gauss curvature provides a way to classify (qualitatively) local surface geometry.

Functions on Surfaces



- Let $f : \Gamma \to \mathbb{R}$ be a function defined on Γ.
- If $(U, \mathbf{X})$ is a local chart, then define $\tilde{f} := f \circ \mathbf{X} : U \to \mathbb{R}$.
- We say f is smooth i.f.f. $\tilde{f}$ is smooth in the usual sense.
- In practice, we first define $\tilde{f} : U \to \mathbb{R}$, then form $f := \tilde{f} \circ \mathbf{X}^{-1}$.

Tangent Vector Fields

- A **tangential vector field** $\mathbf{v} : \Gamma \to \mathbb{R}^3$ is such that $\mathbf{v}(\mathbf{x}) \in T_{\mathbf{x}}(\Gamma)$ for all $\mathbf{x}$ in Γ.
- Using a local chart $(U, \mathbf{X})$, we can find q_1, q_2 such that

$$\mathbf{v} = q_1(s_1, s_2)\partial_{s_1}\mathbf{X}(s_1, s_2) + q_2(s_1, s_2)\partial_{s_2}\mathbf{X}(s_1, s_2), \text{ for all } (s_1, s_2)^\dagger \text{ in } U,$$

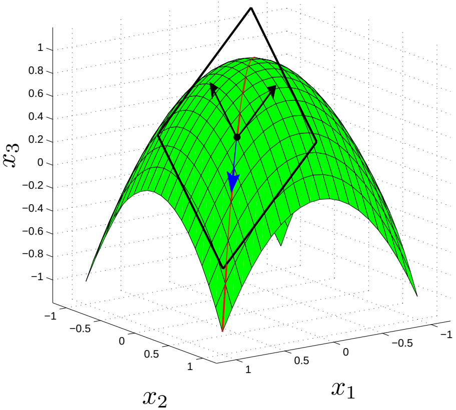
  where $\{\partial_{s_1}\mathbf{X}, \partial_{s_2}\mathbf{X}\}$ is a tangent basis.
- We say $\mathbf{v}$ is smooth, i.f.f. q_1, q_2 are smooth.

Tangential Directional Derivative

- Let $\omega : \Gamma \to \mathbb{R}$ be a surface function.
- Denote the **tangential directional derivative** of ω at P in Γ, in the direction $\mathbf{v}$ in $T_P(\Gamma)$, by $D_{\mathbf{v}}\omega(P)$.

Suppose $\boldsymbol{\alpha}(t)$ is a parameterization of a curve (red) contained in Γ such that $\boldsymbol{\alpha}(0) = P$ and $\boldsymbol{\alpha}'(0) = \mathbf{v}$ (blue), then

$$D_{\mathbf{v}}\omega(P) := \frac{d}{dt}\omega(\boldsymbol{\alpha}(t))\Big|_{t=0}$$



Explicit Calculation

- Introduce a local chart: $(U, \mathbf{X})$.
- Take $\boldsymbol{\alpha}(t) = \mathbf{X} \circ \mathbf{s}(t)$, where $\mathbf{s} : I \to U$ parameterizes a curve in U.
- Define $\tilde{\omega} = \omega \circ \mathbf{X} : U \to \mathbb{R}$.
- Note: $\omega(\boldsymbol{\alpha}(t)) = \omega \circ \mathbf{X} \circ \mathbf{s}(t) = \tilde{\omega} \circ \mathbf{s}(t)$.

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Therefore, the chain rule gives

$$\frac{d}{dt}\omega(\boldsymbol{\alpha}(t)) = \frac{d}{dt}\tilde{\omega}(\mathbf{s}(t)) = (\mathbf{s}'(t) \cdot \nabla_{\mathbf{s}})\tilde{\omega}(\mathbf{s}) = \nabla\tilde{\omega}\mathbf{s}',$$

where $\nabla\tilde{\omega}$ is a 1×2 row vector and $\mathbf{s}'$ is a 2×1 column vector.

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where $\nabla\tilde{\omega}$ is a 1×2 row vector and $\mathbf{s}'$ is a 2×1 column vector.

Expanding further with the metric tensor $g = (\nabla_{\mathbf{s}}\mathbf{X})^{\dagger}(\nabla_{\mathbf{s}}\mathbf{X})$, we obtain

$$\begin{aligned}\frac{d}{dt}\omega(\boldsymbol{\alpha}(t)) &= \nabla\tilde{\omega}g^{-1}g\mathbf{s}', \\ &= \nabla\tilde{\omega}g^{-1}(\nabla_{\mathbf{s}}\mathbf{X})^{\dagger}(\nabla_{\mathbf{s}}\mathbf{X})\mathbf{s}' \\ &= \nabla\tilde{\omega}g^{-1}(\nabla_{\mathbf{s}}\mathbf{X})^{\dagger}\boldsymbol{\alpha}'(t).\end{aligned}$$

Surface Gradient Operator

Hence, we obtain

$$\frac{d}{dt}\omega(\boldsymbol{\alpha}(t))\Big|_{t=0} = \nabla\tilde{\omega}g^{-1}(\nabla_{\mathbf{s}}\mathbf{X})^{\dagger}\boldsymbol{\alpha}'(t)\Big|_{t=0}$$

$$\Rightarrow \quad D_{\mathbf{v}}\omega(P) = \underbrace{\nabla\tilde{\omega}g^{-1}(\nabla_{\mathbf{s}}\mathbf{X})^{\dagger}}_{1\times 3 \text{ row vector}} \cdot \mathbf{v}.$$

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In general,

$$D_{\mathbf{v}}\omega \circ \mathbf{X} = \nabla\tilde{\omega} g^{-1} (\nabla_{\mathbf{s}} \mathbf{X})^{\dagger} \cdot \mathbf{v}, \quad \text{for arbitrary } \mathbf{v},$$

evaluated at $\mathbf{s}$ with $P = \mathbf{X}(\mathbf{s})$.

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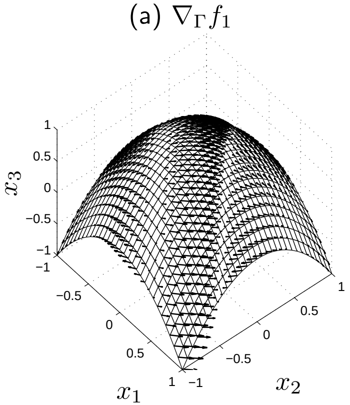
evaluated at $\mathbf{s}$ with $P = \mathbf{X}(\mathbf{s})$.

- Denote the **surface gradient** of ω at P in Γ by $\nabla_{\Gamma}\omega(P)$ in $T_P(\Gamma)$.
- Define it by $\nabla_{\Gamma}\omega(P) \cdot \mathbf{v} = D_{\mathbf{v}}\omega(P)$, for all $\mathbf{v} \in T_P(\Gamma)$.
- Thus,

$$(\nabla_{\Gamma}\omega \circ \mathbf{X}) \cdot \mathbf{v} = D_{\mathbf{v}}\omega \circ \mathbf{X} = \nabla\tilde{\omega} g^{-1} (\nabla_{\mathbf{s}}\mathbf{X})^{\dagger} \cdot \mathbf{v}, \quad \text{for all } \mathbf{v} \in T_{\mathbf{X}(\mathbf{s})}(\Gamma).$$

- Therefore, $\nabla_{\Gamma}\omega \circ \mathbf{X} = \nabla_{\mathbf{s}}\tilde{\omega} g^{-1} (\nabla_{\mathbf{s}}\mathbf{X})^{\dagger}$.

Surface Gradient Example



- If $\boldsymbol{\varphi} = (\varphi_1, \varphi_2, \varphi_3)$, then

$$(\nabla_\Gamma \boldsymbol{\varphi}) \circ \mathbf{X} = \begin{bmatrix} (\nabla_\Gamma \varphi_1) \circ \mathbf{X} \\ (\nabla_\Gamma \varphi_2) \circ \mathbf{X} \\ (\nabla_\Gamma \varphi_3) \circ \mathbf{X} \end{bmatrix}, \quad \text{a } 3 \times 3 \text{ matrix.}$$

Other Surface Operators; Curvatures

Surface Operators:

- Identity map: $\mathrm{id}_\Gamma(\mathbf{x}) = \mathbf{x}$ for all $\mathbf{x}$ in Γ.
- Tangent space projection: $\nabla_\Gamma \mathrm{id}_\Gamma = \mathbf{I} - \boldsymbol{\nu} \otimes \boldsymbol{\nu}$.
- Surface divergence: $\nabla_\Gamma \cdot \boldsymbol{\varphi} = \mathrm{trace}(\nabla_\Gamma \boldsymbol{\varphi})$.
- Surface Laplacian (Laplace-Beltrami): $\Delta_\Gamma \omega := \nabla_\Gamma \cdot \nabla_\Gamma \omega$.

Alternate curvature formulas:

- Curvature vector: $-\Delta_\Gamma \mathrm{id}_\Gamma = \kappa\, \boldsymbol{\nu}$.
- Gauss curvature:

$$\kappa_G = \boldsymbol{\nu} \cdot \frac{\partial_{s_1}\boldsymbol{\nu} \times \partial_{s_2}\boldsymbol{\nu}}{\sqrt{\det(g)}}, \qquad \kappa_G \boldsymbol{\nu} = \frac{\partial_{s_1}\boldsymbol{\nu} \times \partial_{s_2}\boldsymbol{\nu}}{\sqrt{\det(g)}}.$$

- Surface divergence of the normal vector: $\nabla_\Gamma \cdot \boldsymbol{\nu} = \kappa$.

Integration by Parts on Surfaces

- Let Γ be a surface with boundary $\partial\Gamma$.
- $\boldsymbol{\nu}$ is the oriented normal vector of Γ.
- $\boldsymbol{\tau}$ is the positively oriented tangent vector of $\partial\Gamma$.
- Let $\omega : \Gamma \to \mathbb{R}$ be differentiable.
- Integration by parts:

$$\int_{\Gamma} \nabla_{\Gamma}\omega = \int_{\Gamma} \omega\kappa\boldsymbol{\nu} + \int_{\partial\Gamma} \omega(\boldsymbol{\tau} \times \boldsymbol{\nu})$$

- $(\boldsymbol{\tau} \times \boldsymbol{\nu})$ is the “outer normal” of the boundary $\partial\Gamma$.

Another integration by parts formula:

$$\int_{\Gamma} \nabla_{\Gamma}\varphi \cdot \nabla_{\Gamma}\eta = -\int_{\Gamma} \varphi\Delta_{\Gamma}\eta + \int_{\partial\Gamma} \varphi(\boldsymbol{\tau} \times \boldsymbol{\nu}) \cdot \nabla_{\Gamma}\eta,$$

where $\varphi, \eta : \Gamma \to \mathbb{R}$ are differentiable.

Shape Functionals

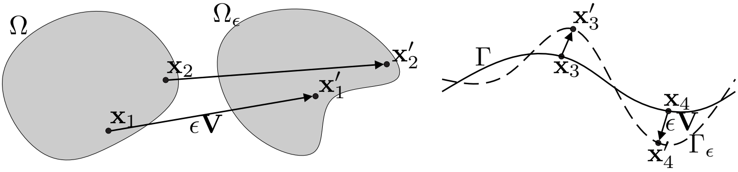
- Recall shape functionals:

$$\mathcal{E}(\Omega) = \int_{\Omega} f(\mathbf{x}, \Omega), \quad \mathcal{J}(\Gamma) = \int_{\Gamma} f(\mathbf{x}, \Omega), \quad \mathcal{B}(\Gamma) = \int_{\Gamma} g(\mathbf{x}, \Gamma).$$

- Note: $\Gamma \subset \Omega$.
- Application: optimization.

$$\Omega^* = \arg\min_{\Omega} \mathcal{E}(\Omega), \quad \Gamma^* = \arg\min_{\Gamma} \mathcal{J}(\Gamma), \quad \Gamma^* = \arg\min_{\Gamma} \mathcal{B}(\Gamma).$$

Perturbing the Domain



Perturbation of the identity:

- Mapping the bulk domain:

$$\mathbf{\Phi}_\epsilon(\mathbf{x}) := \mathbf{x} + \epsilon\mathbf{V}(\mathbf{x}), \quad \text{for all } \mathbf{x} \text{ in } \Omega_{\mathrm{ALL}},$$

  where $\Omega_\epsilon = \mathbf{\Phi}_\epsilon(\Omega)$.

- Mapping an embedded surface:

$$\mathbf{X}_\epsilon \circ \mathbf{X}^{-1}(\mathbf{x}) := \mathbf{x} + \epsilon\mathbf{V}(\mathbf{x}), \quad \text{for all } \mathbf{x} \text{ in } \Gamma \subset \Omega_{\mathrm{ALL}},$$

  where $\Gamma_\epsilon = \mathbf{X}_\epsilon \circ \mathbf{X}^{-1}(\Gamma)$.

Perturbing Functions

- **Material derivative:**

$$\dot{f}(\Omega;\mathbf{V})(\mathbf{x}) \equiv \dot{f}(\mathbf{x}) := \lim_{\epsilon\to 0} \frac{f_\epsilon(\mathbf{\Phi}_\epsilon(\mathbf{x})) - f(\mathbf{x})}{\epsilon}, \quad \text{for all } \mathbf{x} \text{ in } \Omega,$$

- Extend f to all of Ω_{ALL} such that

$$f_\epsilon(\mathbf{\Phi}_\epsilon(\mathbf{x})) = \hat{f}(\epsilon, \mathbf{\Phi}_\epsilon(\mathbf{x})), \quad \text{for all } \mathbf{x} \in \Omega, \quad \epsilon \in [0, \epsilon_{\max}].$$

- Differentiate:

$$\begin{aligned}
\dot{f}(\mathbf{x}) &= \frac{d}{d\epsilon}\hat{f}(\epsilon, \mathbf{\Phi}_\epsilon(\mathbf{x}))\Big|_{\epsilon=0} \\
&= \frac{\partial}{\partial\epsilon}\hat{f}(0,\mathbf{x}) + \nabla\hat{f}(0,\mathbf{x}) \cdot \frac{d}{d\epsilon}\mathbf{\Phi}_\epsilon(\mathbf{x})\Big|_{\epsilon=0} \\
&= \underbrace{\frac{\partial}{\partial\epsilon}\hat{f}(0,\mathbf{x})}_{=:f'(\Omega;\mathbf{V})(\mathbf{x})} + (\mathbf{V}(\mathbf{x}) \cdot \nabla)\underbrace{\hat{f}(0,\mathbf{x})}_{=f(\mathbf{x})}.
\end{aligned}$$

- **Shape derivative:** $f'(\mathbf{x}) \equiv f'(\Omega;\mathbf{V})(\mathbf{x})$.

Perturbing Functions

Relationship between material derivative and shape derivatives:

- Perturbing functions f defined on Ω:

$$\dot{f}(\mathbf{x}) = f'(\mathbf{x}) + \mathbf{V}(\mathbf{x}) \cdot \nabla f(\mathbf{x})$$

- Perturbing functions g defined on Γ:

$$\dot{g}(\mathbf{x}) = g'(\mathbf{x}) + \mathbf{V}(\mathbf{x}) \cdot \nabla_\Gamma g(\mathbf{x})$$

Other examples:

- Local perturbation of Γ:

$$\dot{\mathrm{id}}_\Gamma = \mathbf{V}, \quad \mathrm{id}'_\Gamma = (\mathbf{V} \cdot \boldsymbol{\nu})\boldsymbol{\nu}$$

- Perturb the normal vector:

$$\dot{\boldsymbol{\nu}} = -(\nabla_\Gamma \mathbf{V})^\dagger \boldsymbol{\nu}, \quad \boldsymbol{\nu}' = -\nabla_\Gamma \left(\mathbf{V} \cdot \boldsymbol{\nu}\right)^\dagger$$

- Perturb the summed curvature:

$$\dot{\kappa} = -\boldsymbol{\nu} \cdot (\Delta_\Gamma \mathbf{V}) - 2(\nabla_\Gamma \mathbf{V}) : (\nabla_\Gamma \boldsymbol{\nu}), \quad \kappa' = -\Delta_\Gamma \left(\mathbf{V} \cdot \boldsymbol{\nu}\right)$$

Perturbing Functionals

Consider the perturbed functionals:

$$\mathcal{E}_\epsilon = \int_{\Omega_\epsilon} f(\Omega_\epsilon), \quad \mathcal{J}_\epsilon = \int_{\Gamma_\epsilon} f(\Omega_\epsilon), \quad \mathcal{B}_\epsilon = \int_{\Gamma_\epsilon} g(\Gamma_\epsilon), \quad \text{for all } \epsilon \geq 0,$$

and define the corresponding shape perturbations:

$$\begin{aligned}
\delta\mathcal{E}(\Omega) \cdot \mathbf{V} \equiv \delta\mathcal{E}(\Omega; \mathbf{V}) &:= \frac{d}{d\epsilon}\mathcal{E}_\epsilon\Big|_{\epsilon=0^+}, \\
\delta\mathcal{J}(\Gamma) \cdot \mathbf{V} \equiv \delta\mathcal{J}(\Gamma; \mathbf{V}) &:= \frac{d}{d\epsilon}\mathcal{J}_\epsilon\Big|_{\epsilon=0^+}, \\
\delta\mathcal{B}(\Gamma) \cdot \mathbf{V} \equiv \delta\mathcal{B}(\Gamma; \mathbf{V}) &:= \frac{d}{d\epsilon}\mathcal{B}_\epsilon\Big|_{\epsilon=0^+}.
\end{aligned}$$

Perturbing Functionals

$$\delta\mathcal{E}(\Omega;\mathbf{V}) = \int_\Omega \dot{f}(\Omega;\mathbf{V}) + \int_\Omega f(\Omega)(\nabla\cdot\mathbf{V}) = \overbrace{\int_\Omega f'(\Omega;\mathbf{V}) + \int_{\partial\Omega} f(\Omega)(\mathbf{V}\cdot\boldsymbol{\nu})}^{\text{recall intro. example}},$$

$$\begin{aligned}
\delta\mathcal{J}(\Gamma;\mathbf{V}) &= \int_\Gamma \dot{f}(\Omega;\mathbf{V}) + f(\nabla_\Gamma\cdot\mathbf{V}) \\
&= \int_\Gamma f'(\Omega;\mathbf{V}) + (\mathbf{V}\cdot\nabla)f + f(\nabla_\Gamma\cdot\mathbf{V}) \\
&= \int_\Gamma f'(\Omega;\mathbf{V}) + \left[(\boldsymbol{\nu}\cdot\nabla)f + f\kappa\right](\mathbf{V}\cdot\boldsymbol{\nu}) + \int_{\partial\Gamma} f(\boldsymbol{\tau}\times\boldsymbol{\nu})\cdot\mathbf{V},
\end{aligned}$$

$$\begin{aligned}
\delta\mathcal{B}(\Gamma;\mathbf{V}) &= \int_\Gamma \dot{g}(\Gamma;\mathbf{V}) + g(\nabla_\Gamma\cdot\mathbf{V}) \\
&= \int_\Gamma g'(\Gamma;\mathbf{V}) + (\mathbf{V}\cdot\nabla_\Gamma)g + g(\nabla_\Gamma\cdot\mathbf{V}) \\
&= \int_\Gamma g'(\Gamma;\mathbf{V}) + g\kappa(\mathbf{V}\cdot\boldsymbol{\nu}) + \int_{\partial\Gamma} g(\boldsymbol{\tau}\times\boldsymbol{\nu})\cdot\mathbf{V}.
\end{aligned}$$

Structure Theorem

- Hadamard-Zolésio structure theorem.
- Ω is a "flat" domain.
- Let $\mathcal{J} = \mathcal{J}(\Omega)$ be a generic shape functional, whose shape perturbation exists.
- If everything is sufficiently smooth, then one can always write

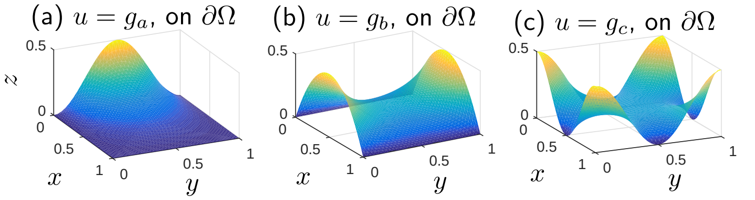
$$\delta\mathcal{J}(\Omega; \mathbf{V}) = \int_{\partial\Omega} \eta(\mathbf{V} \cdot \boldsymbol{\nu}),$$

  for some function η in $L^1(\partial\Omega)$.
- Example:

$$\delta\mathcal{E}(\Omega; \mathbf{V}) = \int_{\Omega} f'(\Omega; \mathbf{V}) + \int_{\partial\Omega} f(\Omega)(\mathbf{V} \cdot \boldsymbol{\nu}).$$

- Rewriting $\int_{\Omega} f'(\Omega; \mathbf{V})$ as an integral over $\partial\Omega$ requires using an **adjoint** PDE.

Minimal Surfaces



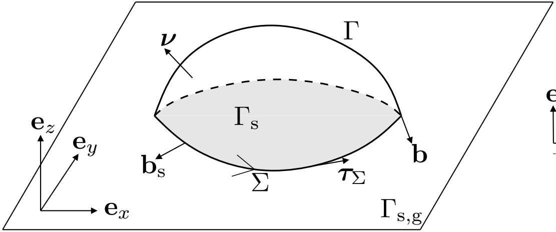
- Let Γ be a surface with boundary $\partial\Gamma \equiv \Sigma$.
- Perimeter functional: $\mathcal{J}(\Gamma) = \int_{\Gamma} 1 \, dS$.
- What is the first order optimality condition?
- Apply shape perturbation formula with $f = 1$:

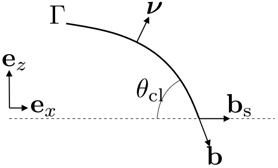
$$\begin{aligned} \delta\mathcal{J}(\Gamma; \mathbf{V}) &= \int_{\Gamma} f' + \left[(\boldsymbol{\nu} \cdot \nabla) f + f\kappa \right] (\mathbf{V} \cdot \boldsymbol{\nu}) + \int_{\Sigma} f (\boldsymbol{\tau} \times \boldsymbol{\nu}) \cdot \mathbf{V}, \\ &= \int_{\Gamma} \kappa \boldsymbol{\nu} \cdot \mathbf{V} = 0, \end{aligned}$$

for all smooth perturbations $\mathbf{V}$ that *vanish* on Σ.

- First order condition is: $\kappa = 0$.

Surface Tension





- Let γ be a surface tension coefficient.
- Consider the surface energy functional: $\mathcal{J}(\Gamma) = \int_\Gamma \gamma \, dS(\mathbf{x})$.
- Differentiating the energy gives the "force":

$$\delta\mathcal{J}(\Gamma; \mathbf{V}) = \int_\Gamma \gamma\kappa\boldsymbol{\nu} \cdot \mathbf{V} + \int_\Sigma \gamma\mathbf{b} \cdot \mathbf{V},$$

  where $\mathbf{V}$ is a perturbation of the surface Γ. Note: $\mathbf{b} = \boldsymbol{\tau}_\Sigma \times \boldsymbol{\nu}$.
- $\delta\mathcal{J}(\Gamma; \mathbf{V})$ is the relative force exerted by surface tension against deforming the surface by $\mathbf{V}$.
- Integral over Σ are the contact line forces.

Shape Optimization

- Consider a shape functional $\mathcal{J} = \mathcal{J}(\Gamma)$ defined over a set of admissible shapes $\mathcal{U}$.
- The optimization problem is:

$$\text{find } \Gamma^* \in \mathcal{U}, \text{ such that } \mathcal{J}(\Gamma^*) = \min_{\Gamma \in \mathcal{U}} \mathcal{J}(\Gamma).$$

- Can we evolve $\Gamma = \Gamma(t)$ with a "velocity field" such that

$$\mathcal{J}(\Gamma(t_2)) < \mathcal{J}(\Gamma(t_1)), \text{ whenever } t_1 < t_2.$$

- Note: "time" here is a pseudotime that corresponds to our flow "velocity."

Variational Problem

- Define a "velocity" space:

$$\mathbb{V}(\Gamma) = \left\{ \mathbf{V} : \int_{\Gamma} |\mathbf{V}|^2 < \infty \right\}, \text{ with norm } \|\mathbf{V}\|_{\mathbb{V}(\Gamma)} := \left(\int_{\Gamma} |\mathbf{V}|^2 \right)^{1/2}$$

- Define a bilinear form $b : \mathbb{V}(\Gamma) \times \mathbb{V}(\Gamma) \to \mathbb{R}$ such that $b(\mathbf{V}, \mathbf{Y}) = \int_{\Gamma} \mathbf{V} \cdot \mathbf{Y}$.
- Note that $\|\mathbf{V}\|_{\mathbb{V}(\Gamma)} = \sqrt{b(\mathbf{V}, \mathbf{V})}$.
- We now **define** the velocity field as follows: at each time $t \geq 0$, find $\mathbf{V}(t)$ in $\mathbb{V}(\Gamma(t))$ that solves the following variational problem:

$$b(\mathbf{V}(t), \mathbf{Y}) = -\delta \mathcal{J}(\Gamma(t); \mathbf{Y}), \text{ for all } \mathbf{Y} \in \mathbb{V}(\Gamma(t)).$$

- This ensures we *decrease* the energy because

$$\delta \mathcal{J}(\Gamma(t); \mathbf{V}(t)) = -b(\mathbf{V}(t), \mathbf{V}(t)) = -\|\mathbf{V}(t)\|^2_{\mathbb{V}(\Gamma)} < 0.$$

L^2-Gradient Descent

Discretize time:

- Start with an initial domain Γ^0.
- **FOR** $i = 0, 1, 2, ...$, find $\mathbf{V}^i$ in $\mathbb{V}(\Gamma^i)$ such that

$$b(\mathbf{V}^i, \mathbf{Y}) = -\delta \mathcal{J}(\Gamma^i; \mathbf{Y}), \text{ for all } \mathbf{Y} \in \mathbb{V}(\Gamma^i).$$

- Define perturbation of the identity:

$$\mathbf{X}_{\Delta t} \circ (\mathbf{X}^i)^{-1}(\mathbf{x}) := \mathrm{id}_{\Gamma^i}(\mathbf{x}) + \Delta t \mathbf{V}^i(\mathbf{x}), \quad \text{for all } \mathbf{x} \text{ in } \Gamma^i.$$

  where $\mathbf{X}^i$ is a parameterization of Γ^i, and Δt is a "time-step".
- Update the domain: $\Gamma^{i+1} = \mathbf{X}_{\Delta t} \circ (\mathbf{X}^i)^{-1}(\Gamma^i)$.
- If the time step Δt is small enough, then the sequence $\{\mathcal{J}(\Gamma^i)\}_{i \geq 0}$ is decreasing, i.e.

$$\mathcal{J}(t_0) > \mathcal{J}(t_1) > \mathcal{J}(t_2) > \cdots > \mathcal{J}(t_i) > \mathcal{J}(t_{i+1}) > \cdots$$

- Choosing a different space $\mathbb{V}(\Gamma)$ can improve the convergence rate.

Mean Curvature Flow

- Assume Γ is a closed surface.
- Consider the perimeter functional: $\mathcal{J}(\Gamma) = \int_{\Gamma} 1 \, dS(\mathbf{x})$.
- For each $t \geq 0$, find $\mathbf{V}(t)$ such that

$$\int_{\Gamma(t)} \mathbf{V}(t) \cdot \mathbf{Y} = -\delta \mathcal{J}(\Gamma(t); \mathbf{Y}) = -\int_{\Gamma(t)} \kappa(t) \boldsymbol{\nu}(t) \cdot \mathbf{Y},$$

for all smooth perturbations $\mathbf{Y}$.

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  for all smooth perturbations $\mathbf{Y}$.
- Continuing, we get

$$\int_{\Gamma(t)} \left[\mathbf{V}(t) + \kappa(t) \boldsymbol{\nu}(t) \right] \cdot \mathbf{Y} = 0, \quad \text{for all smooth } \mathbf{Y}.$$

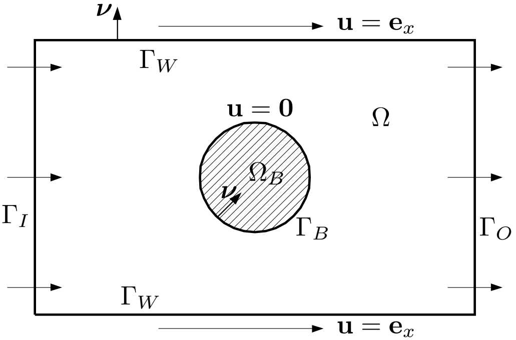
- Therefore, $\mathbf{V}(t, \mathbf{x}) = -\kappa(t, \mathbf{x}) \boldsymbol{\nu}(t, \mathbf{x})$, for all $\mathbf{x} \in \Gamma(t)$.
- The surface $\Gamma(t)$ moves with normal velocity:

$$\mathbf{V} \cdot \boldsymbol{\nu} = -\kappa.$$

- Mean curvature flow is the L^2-gradient flow of perimeter.

Shape Optimization Example: Drag Minimization

- Define $\Omega = \Omega_{\text{ALL}} \setminus \Omega_B$.



Navier-Stokes Equations:

$$
\begin{aligned}
(\mathbf{u} \cdot \nabla)\mathbf{u} - \nabla \cdot \boldsymbol{\sigma} &= \mathbf{0}, \text{ in } \Omega, \\
\nabla \cdot \mathbf{u} &= 0, \text{ in } \Omega, \\
\mathbf{u} &= \mathbf{0}, \text{ on } \Gamma_B, \\
\mathbf{u} &= \mathbf{e}_x, \text{ on } \Gamma_I, \\
\mathbf{u} &= \mathbf{e}_x, \text{ on } \Gamma_W, \\
\boldsymbol{\sigma}\boldsymbol{\nu} &= \mathbf{0}, \text{ on } \Gamma_O.
\end{aligned}
$$

- Cost functional: $\mathcal{J}(\Omega) = -\mathbf{e}_x \cdot \int_{\Gamma_B} \boldsymbol{\sigma}(\mathbf{u}, p)\boldsymbol{\nu}$ (drag force).
- Newtonian fluid: $\boldsymbol{\sigma}(\mathbf{u}, p) := -pI + \frac{2}{\text{Re}} D(\mathbf{u})$, $D(\mathbf{u}) := \frac{\nabla \mathbf{u} + (\nabla \mathbf{u})^{\dagger}}{2}$.
- Reynolds number: $\text{Re} = \frac{\rho U_0 L}{\mu}$.

Rewrite Cost Functional

$$\text{Define } \boldsymbol{\varphi} := \mathbf{u} - \mathbf{e}_x : \quad \Rightarrow \quad \begin{aligned} \nabla \cdot \boldsymbol{\varphi} &= 0, \text{ in } \Omega, \\ \boldsymbol{\varphi} &= -\mathbf{e}_x, \text{ on } \Gamma_B, \\ \boldsymbol{\varphi} &= \mathbf{0}, \text{ on } \Gamma_I \cup \Gamma_W. \end{aligned}$$

- Manipulate the cost:

$$\begin{aligned} \mathcal{J}(\Omega) &= -\mathbf{e}_x \cdot \int_{\Gamma_B} \boldsymbol{\sigma}(\mathbf{u}, p)\boldsymbol{\nu} = \int_{\Gamma_B} \boldsymbol{\varphi} \cdot \boldsymbol{\sigma}(\mathbf{u}, p)\boldsymbol{\nu} \\ &= \int_{\partial\Omega} \boldsymbol{\nu} \cdot \boldsymbol{\sigma}\boldsymbol{\varphi} = \int_{\Omega} \nabla \cdot (\boldsymbol{\sigma}\boldsymbol{\varphi}) = \int_{\Omega} \left\{ [\nabla \cdot \boldsymbol{\sigma}] \cdot \boldsymbol{\varphi} + \boldsymbol{\sigma} : \nabla \boldsymbol{\varphi} \right\} \\ &= \int_{\Omega} \left\{ [\nabla \cdot \boldsymbol{\sigma}] \cdot \boldsymbol{\varphi} - p\mathbf{I} : \nabla \mathbf{u} + \frac{2}{\mathrm{Re}} D(\mathbf{u}) : \nabla \mathbf{u} \right\} \\ &= \int_{\Omega} [(\mathbf{u} \cdot \nabla)\mathbf{u}] \cdot \boldsymbol{\varphi} + \frac{2}{\mathrm{Re}} \int_{\Omega} D(\mathbf{u}) : D(\mathbf{u}) \end{aligned}$$

- Perturbing bulk domains is usually *easier* than surface domains.

Differentiate The Cost

$$\mathcal{J}(\Omega) = \int_{\Omega} [(\mathbf{u} \cdot \nabla)\mathbf{u}] \cdot \boldsymbol{\varphi} + \frac{2}{\mathrm{Re}} \int_{\Omega} D(\mathbf{u}) : D(\mathbf{u})$$

Apply shape perturbation formula:

$$\begin{aligned}\delta\mathcal{J}(\Omega; \mathbf{V}) = \int_{\Omega} \left[(\mathbf{u}' \cdot \nabla)\mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u}'\right] \cdot \boldsymbol{\varphi} + \int_{\Omega} [(\mathbf{u} \cdot \nabla)\mathbf{u}] \cdot \boldsymbol{\varphi}' \\ + \int_{\partial\Omega} (\mathbf{V} \cdot \boldsymbol{\nu})[(\mathbf{u} \cdot \nabla)\mathbf{u}] \cdot \boldsymbol{\varphi} + \\ + \frac{4}{\mathrm{Re}} \int_{\Omega} D(\mathbf{u}') : D(\mathbf{u}) + \frac{2}{\mathrm{Re}} \int_{\partial\Omega} (\mathbf{V} \cdot \boldsymbol{\nu})|D(\mathbf{u})|^2\end{aligned}$$

Differentiate The Cost

$$\mathcal{J}(\Omega) = \int_{\Omega} [(\mathbf{u} \cdot \nabla)\mathbf{u}] \cdot \boldsymbol{\varphi} + \frac{2}{\mathrm{Re}} \int_{\Omega} D(\mathbf{u}) : D(\mathbf{u})$$

Apply shape perturbation formula:

$$\begin{aligned}
\delta\mathcal{J}(\Omega; \mathbf{V}) = & \int_{\Omega} \left[(\mathbf{u}' \cdot \nabla)\mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u}'\right] \cdot \boldsymbol{\varphi} + \int_{\Omega} [(\mathbf{u} \cdot \nabla)\mathbf{u}] \cdot \boldsymbol{\varphi}' \\
& + \int_{\partial\Omega} (\mathbf{V} \cdot \boldsymbol{\nu})[(\mathbf{u} \cdot \nabla)\mathbf{u}] \cdot \boldsymbol{\varphi} + \\
& + \frac{4}{\mathrm{Re}} \int_{\Omega} D(\mathbf{u}') : D(\mathbf{u}) + \frac{2}{\mathrm{Re}} \int_{\partial\Omega} (\mathbf{V} \cdot \boldsymbol{\nu}) |D(\mathbf{u})|^2 \\
= & \int_{\Omega} \left[(\mathbf{u}' \cdot \nabla)\mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u}'\right] \cdot \boldsymbol{\varphi} + \frac{2}{\mathrm{Re}} \int_{\Omega} D(\mathbf{u}') : \nabla\boldsymbol{\varphi} \\
& + \int_{\Omega} [(\mathbf{u} \cdot \nabla)\mathbf{u}] \cdot \mathbf{u}' + \frac{2}{\mathrm{Re}} \int_{\Omega} D(\mathbf{u}) : \nabla\mathbf{u}' + \\
& + \int_{\Gamma_B} (\mathbf{V} \cdot \boldsymbol{\nu})[(\mathbf{u} \cdot \nabla)\mathbf{u}] \cdot \boldsymbol{\varphi} + \frac{2}{\mathrm{Re}} \int_{\Gamma_B} (\mathbf{V} \cdot \boldsymbol{\nu}) |D(\mathbf{u})|^2,
\end{aligned}$$

where we used the fact that $\mathbf{V} = \mathbf{0}$ on $\partial\Omega \setminus \Gamma_B$.

Differentiate The PDE

$$
\begin{aligned}
\delta\mathcal{J}(\Gamma_B;\mathbf{V}) = &\int_\Omega \left[(\mathbf{u}'\cdot\nabla)\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u}'\right]\cdot\boldsymbol{\varphi} + \int_\Omega \boldsymbol{\sigma}(\mathbf{u}',p') : \nabla\boldsymbol{\varphi} \\
&+ \int_\Omega [(\mathbf{u}\cdot\nabla)\mathbf{u}]\cdot\mathbf{u}' + \int_\Omega \boldsymbol{\sigma}(\mathbf{u},p) : \nabla\mathbf{u}' + \\
&+ \int_{\Gamma_B} (\mathbf{V}\cdot\boldsymbol{\nu})[(\mathbf{u}\cdot\nabla)\mathbf{u}]\cdot\boldsymbol{\varphi} + \frac{2}{\mathrm{Re}}\int_{\Gamma_B} (\mathbf{V}\cdot\boldsymbol{\nu})|D(\mathbf{u})|^2
\end{aligned}
$$

Differentiate The PDE

$$\delta \mathcal{J}(\Gamma_B; \mathbf{V}) = \int_\Omega \left[(\mathbf{u}' \cdot \nabla)\mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u}' \right] \cdot \boldsymbol{\varphi} + \int_\Omega \boldsymbol{\sigma}(\mathbf{u}', p') : \nabla \boldsymbol{\varphi}$$

$$+ \int_\Omega [(\mathbf{u} \cdot \nabla)\mathbf{u}] \cdot \mathbf{u}' + \int_\Omega \boldsymbol{\sigma}(\mathbf{u}, p) : \nabla \mathbf{u}' +$$

$$+ \int_{\Gamma_B} (\mathbf{V} \cdot \boldsymbol{\nu})[(\mathbf{u} \cdot \nabla)\mathbf{u}] \cdot \boldsymbol{\varphi} + \frac{2}{\mathrm{Re}} \int_{\Gamma_B} (\mathbf{V} \cdot \boldsymbol{\nu}) |D(\mathbf{u})|^2$$

int. by parts

$$= \int_\Omega \left[(\mathbf{u}' \cdot \nabla)\mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u}' - \nabla \cdot \boldsymbol{\sigma}' \right] \cdot \boldsymbol{\varphi} + \int_{\partial\Omega} \boldsymbol{\sigma}' \boldsymbol{\nu} \cdot \boldsymbol{\varphi}$$

$$+ \int_\Omega \left[(\mathbf{u} \cdot \nabla)\mathbf{u} - \nabla \cdot \boldsymbol{\sigma} \right] \cdot \mathbf{u}' + \int_{\partial\Omega} \boldsymbol{\sigma} \boldsymbol{\nu} \cdot \mathbf{u}' +$$

$$+ \int_{\Gamma_B} (\mathbf{V} \cdot \boldsymbol{\nu})[(\mathbf{u} \cdot \nabla)\mathbf{u}] \cdot \boldsymbol{\varphi} + \frac{2}{\mathrm{Re}} \int_{\Gamma_B} (\mathbf{V} \cdot \boldsymbol{\nu}) |D(\mathbf{u})|^2$$

$$\begin{aligned}
(\mathbf{u} \cdot \nabla)\mathbf{u} - \nabla \cdot \boldsymbol{\sigma} &= \mathbf{0}, \text{ in } \Omega, \\
\nabla \cdot \mathbf{u} &= 0, \text{ in } \Omega, \\
\mathbf{u} &= \mathbf{0}, \text{ on } \Gamma_B, \\
\mathbf{u} &= \mathbf{e}_x, \text{ on } \Gamma_I \cup \Gamma_W, \\
\boldsymbol{\sigma}\boldsymbol{\nu} &= \mathbf{0}, \text{ on } \Gamma_O.
\end{aligned}$$

$$\begin{aligned}
(\mathbf{u}' \cdot \nabla)\mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u}' - \nabla \cdot \boldsymbol{\sigma}' &= \mathbf{0}, \text{ in } \Omega, \\
\nabla \cdot \mathbf{u}' &= 0, \text{ in } \Omega, \\
\mathbf{u}' &= ??, \text{ on } \Gamma_B, \\
\mathbf{u}' &= \mathbf{0}, \text{ on } \Gamma_I \cup \Gamma_W, \\
\boldsymbol{\sigma}'\boldsymbol{\nu} &= \mathbf{0}, \text{ on } \Gamma_O.
\end{aligned}$$

Use The Adjoint Variable

- The shape perturbation reduces to

$$\delta \mathcal{J}(\Gamma_B; \mathbf{V}) = \int_{\Gamma_B} \boldsymbol{\sigma}' \boldsymbol{\nu} \cdot \boldsymbol{\varphi} + \int_{\Gamma_B} \boldsymbol{\sigma} \boldsymbol{\nu} \cdot \mathbf{u}' + \frac{2}{\mathrm{Re}} \int_{\Gamma_B} (\mathbf{V} \cdot \boldsymbol{\nu}) |D(\mathbf{u})|^2$$

Use The Adjoint Variable

- The shape perturbation reduces to

$$\delta \mathcal{J}(\Gamma_B; \mathbf{V}) = \int_{\Gamma_B} \boldsymbol{\sigma}' \boldsymbol{\nu} \cdot \boldsymbol{\varphi} + \int_{\Gamma_B} \boldsymbol{\sigma} \boldsymbol{\nu} \cdot \mathbf{u}' + \frac{2}{\mathrm{Re}} \int_{\Gamma_B} (\mathbf{V} \cdot \boldsymbol{\nu}) |D(\mathbf{u})|^2$$

- Next, we need the adjoint PDE, i.e. find $(\mathbf{r}, \pi)$ such that:

$$\begin{aligned} -[\nabla \mathbf{r}]^{\dagger} \mathbf{u} - (\mathbf{u} \cdot \nabla) \mathbf{r} - \nabla \cdot S(\mathbf{r}, \pi) &= \mathbf{0}, \text{ in } \Omega, \\ \nabla \cdot \mathbf{r} &= 0, \text{ in } \Omega, \\ \mathbf{r} = \boldsymbol{\varphi} &= -\mathbf{e}_x, \text{ on } \Gamma_B, \\ \mathbf{r} &= \mathbf{0}, \text{ on } \Gamma_I \cup \Gamma_W, \\ S\boldsymbol{\nu} &= \mathbf{0}, \text{ on } \Gamma_O, \end{aligned}$$

where $S(\mathbf{r}, \pi) = -\pi \mathbf{I} + \frac{2}{\mathrm{Re}} D(\mathbf{r})$.

- Thus, after lots of integration by parts, etc.,

$$\delta \mathcal{J}(\Gamma_B; \mathbf{V}) = \int_{\Gamma_B} S\boldsymbol{\nu} \cdot \mathbf{u}' + \int_{\Gamma_B} \boldsymbol{\sigma} \boldsymbol{\nu} \cdot \mathbf{u}' + \frac{2}{\mathrm{Re}} \int_{\Gamma_B} (\mathbf{V} \cdot \boldsymbol{\nu}) |D(\mathbf{u})|^2$$

Simplify

- Since $\mathbf{u} = \mathbf{0}$ on Γ_B, regardless of the shape of Γ_B, we have that

$$\dot{\mathbf{u}} = \mathbf{0}, \text{ on } \Gamma_B.$$

- Therefore, $\mathbf{u}' = -(\mathbf{V} \cdot \nabla)\mathbf{u} = -[\nabla \mathbf{u}]\mathbf{V}, \text{ on } \Gamma_B$.
- Hence, the shape perturbation simplifies to

$$\begin{aligned}
\delta \mathcal{J}(\Gamma_B; \mathbf{V}) &= -\int_{\Gamma_B} (S\boldsymbol{\nu} + \boldsymbol{\sigma}\boldsymbol{\nu}) \cdot [\nabla \mathbf{u}]\mathbf{V} + \frac{2}{\mathrm{Re}} \int_{\Gamma_B} (\mathbf{V} \cdot \boldsymbol{\nu}) |D(\mathbf{u})|^2 \\
&= -\int_{\Gamma_B} \left\{ (S\boldsymbol{\nu} + \boldsymbol{\sigma}\boldsymbol{\nu}) \cdot [\nabla \mathbf{u}]\boldsymbol{\nu} \right\} (\mathbf{V} \cdot \boldsymbol{\nu}) \\
&\qquad + \frac{2}{\mathrm{Re}} \int_{\Gamma_B} (\mathbf{V} \cdot \boldsymbol{\nu}) |D(\mathbf{u})|^2 \\
&= \int_{\Gamma_B} \eta (\mathbf{V} \cdot \boldsymbol{\nu}).
\end{aligned}$$

- This satisfies the structure theorem.
- η is sometimes called the **shape gradient**.

Shape Gradient Descent

- Start with an initial domain Γ_B^i.
- **FOR** $i = 0, 1, 2, ...$, do the following.
- Solve for $(\mathbf{u}, p)$ and $(\mathbf{r}, \pi)$ on Ω^i.
- Evaluate η^i.
- Find $\mathbf{V}^i$ in $\mathbb{V}(\Gamma_B^i)$ such that

$$b(\mathbf{V}^i, \mathbf{Y}) = -\delta\mathcal{J}(\Gamma_B^i; \mathbf{Y}), \text{ for all } \mathbf{Y} \in \mathbb{V}(\Gamma_B^i).$$

- Update the domain using $\mathbf{V}^i$ to obtain Γ_B^{i+1} (**line-search!**).
- Choice of $\mathbb{V}(\Gamma_B)$ can improve the convergence rate, e.g.

$$\mathbb{V}(\Gamma_B) = \left\{ \mathbf{V} : \int_{\Gamma_B} |\mathbf{V}|^2 + \int_{\Gamma_B} |\nabla_{\Gamma_B}\mathbf{V}|^2 < \infty \right\}.$$

Min Drag Movie

Remarks

Issues we did not talk about:

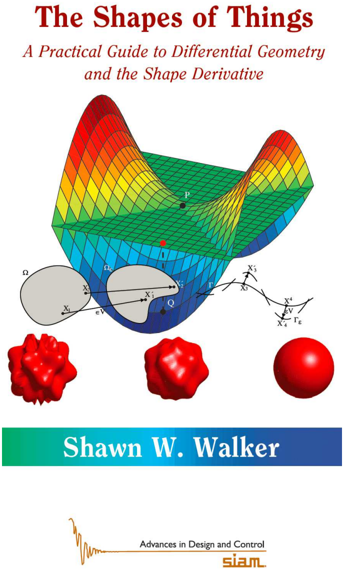
- *Existence* of a minimizer; mostly the same as usual.
- Can *restrict* the admissible set to give existence.
- In general, can be quite difficult. Even the minimal surface problem is not completely understood.
- *Lower-semicontinuity* of the functional.
- Optimize-then-discretize Vs. Discretize-then-optimize, e.g. the issue of *inconsistent* gradients.
- Is the solution *regular* enough?

Book On Shape Differential Calculus

- Moving interfaces often involve curvature.
- Can be understood in the context of shape differentiation.
- Shape gradients necessary for *shape optimization*.

SIAM Book Series: *Advances in Design and Control*, vol 28, July 2015.

- Book is written at the undergraduate level.
- Also useful for first year graduate students.
- First book to make this material accessible to a wider audience.



Summary

- Provided a "crash course" on differential geometry.
- Defined surface derivatives.
- Introduced shape differential calculus.
- Brief introduction to gradient flows.
- Worked an example on drag minimization.

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