

# Introduction to Shape Optimization

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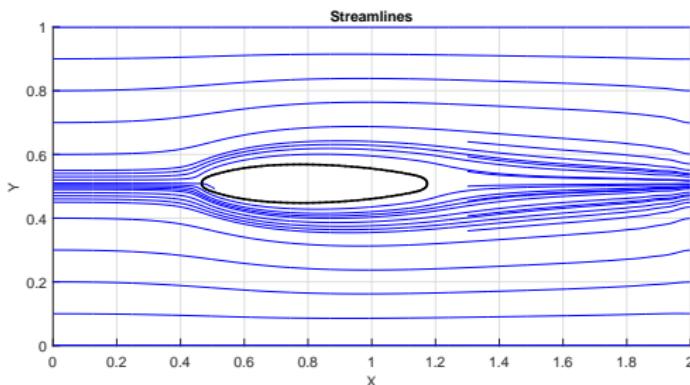
Frontiers in PDE-constrained Optimization

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- 2 Differential Geometry
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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.



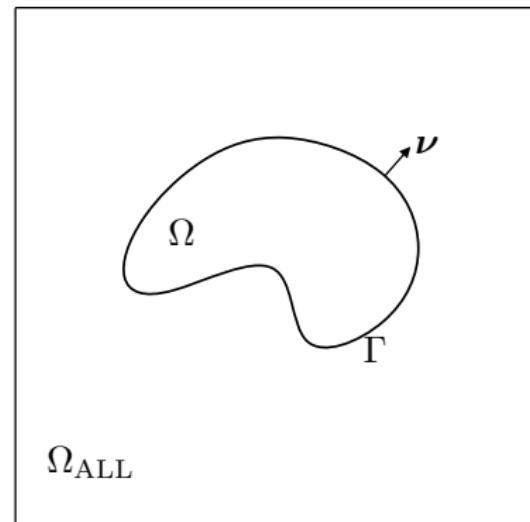
# Mathematical Statement

## Admissible Set:

- Let  $\Omega_{\text{ALL}}$  be a “hold-all” domain.
- Optimization variable is  $\Omega$  or  $\Gamma$ .
- Denote the admissible set by  $\mathcal{U}$ .
- $\mathcal{U}$  should have a *compactness* property.

## Cost Functional:

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



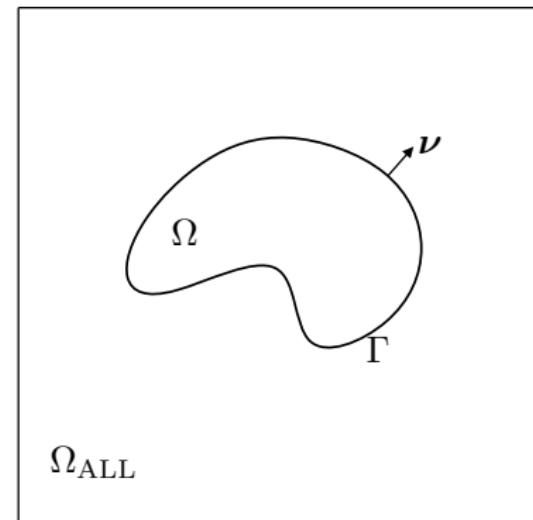
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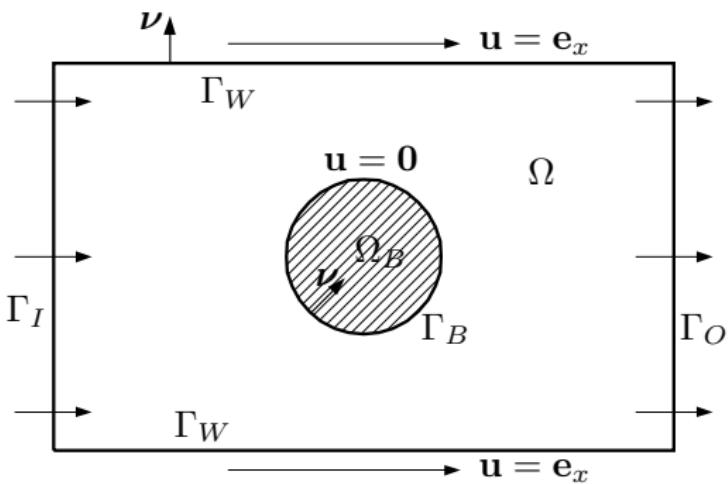
## Optimization Problem:

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

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

# Shape Optimization Example: Drag Minimization

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

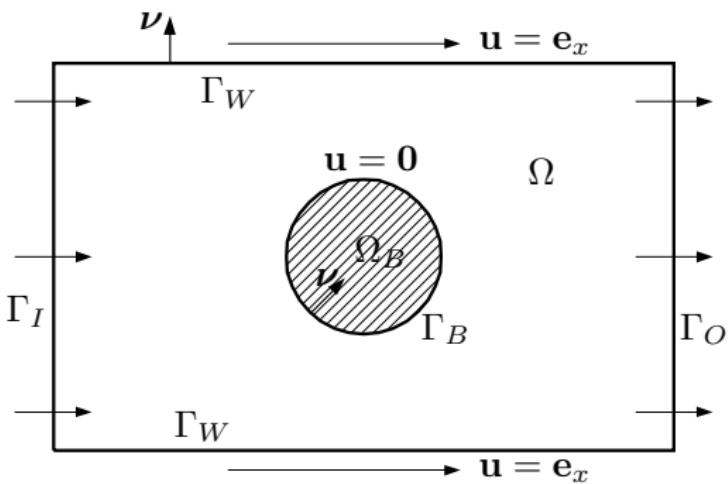


Navier-Stokes Equations:

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

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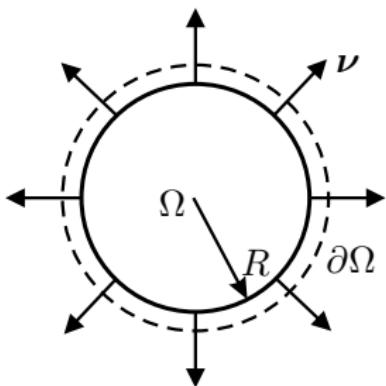


Navier-Stokes Equations:

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 \mathbf{u} &= \mathbf{e}_x, \quad \text{on } \Gamma_W, \\
 \boldsymbol{\sigma} \nu &= \mathbf{0}, \quad \text{on } \Gamma_O.
 \end{aligned}$$

- Cost functional:  $\mathcal{J}(\Omega) = -\mathbf{e}_x \cdot \int_{\Gamma_B} \boldsymbol{\sigma}(\mathbf{u}, p) \nu$  (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:  $\text{Re} = \frac{\rho U_0 L}{\mu}$ .

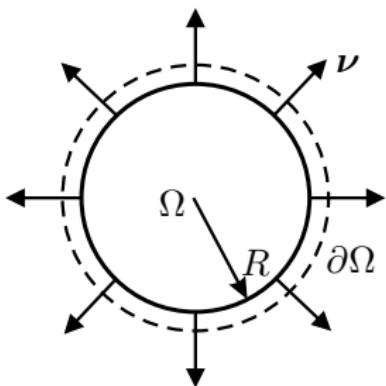
# Shape Sensitivity: Simple Example



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

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

# Shape Sensitivity: Simple Example



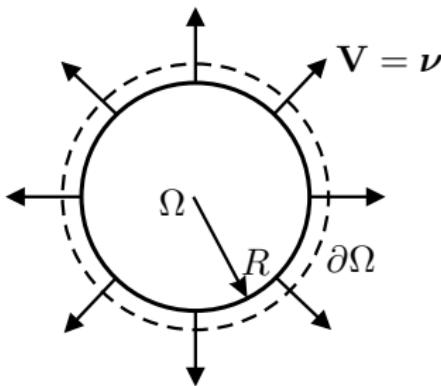
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- What is the *sensitivity* of  $\mathcal{J}$  with respect to changing  $R$ ?
- Polar coordinates:  $\mathcal{J} = \int_0^{2\pi} \int_0^R f(r, \theta; R) r dr d\theta$ .
- Differentiate:

$$\begin{aligned} \frac{d}{dR} \mathcal{J} &= \int_0^{2\pi} \left( \frac{d}{dR} \int_0^R f(r, \theta; R) r dr \right) d\theta \\ &= \int_0^{2\pi} \int_0^R f'(r, \theta; R) r dr d\theta + \int_0^{2\pi} f(R, \theta; R) R d\theta. \end{aligned}$$

# Shape Sensitivity: Simple Example

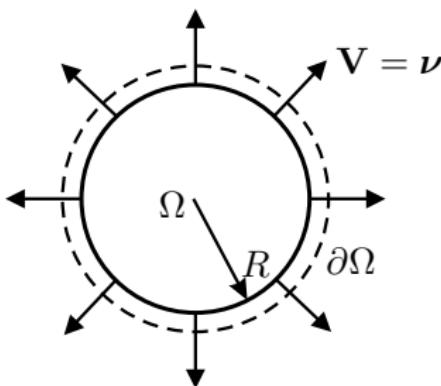


- Change back to Cartesian coordinates:

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

where  $f'$  is the derivative with respect to  $R$ .

# Shape Sensitivity: Simple Example



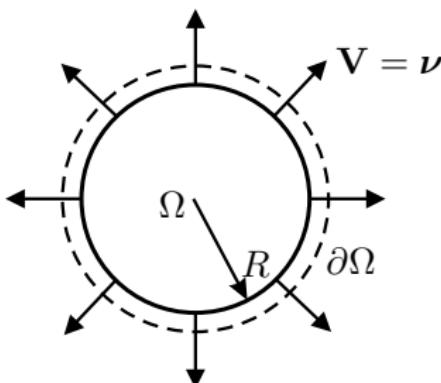
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where  $f'$  is the derivative with respect to  $R$ .

- Indeed,  $f'$  is actually the derivative with respect to deforming  $\Omega$ !
- Here,  $\Omega$  is deformed by the “flow field”  $V = \nu$ .

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- Indeed,  $f'$  is actually the derivative with respect to deforming  $\Omega$ !
- Here,  $\Omega$  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  $\Omega$ .

# 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  $\Omega$ ,  $|\Gamma|$  is the surface area of  $\Gamma$ , and  $|\Sigma|$  is the arc-length of the curve  $\Sigma$ .

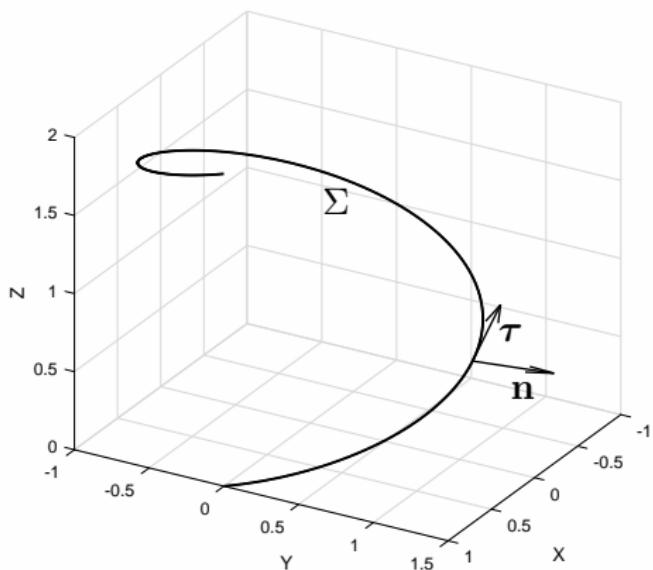
# Parametric Curves

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

$$\alpha(t) = \int_0^t |\alpha'(s)| ds.$$

- Derivative with respect to arc-length  $\alpha$ :

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



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

# Parametric Curves

- Tangent vector:

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

- Curvature vector:

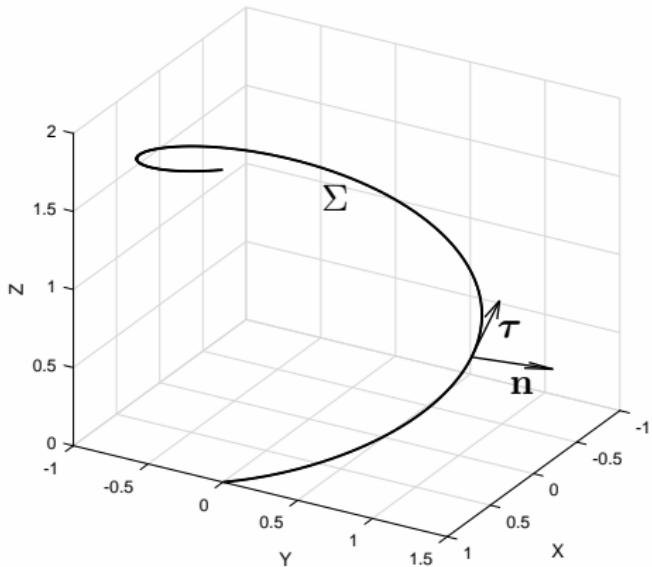
$$k\mathbf{n} := -\frac{d^2\alpha}{d\alpha^2} = -\frac{d\tau}{d\alpha},$$

where  $\mathbf{n}$  is the unit normal vector.

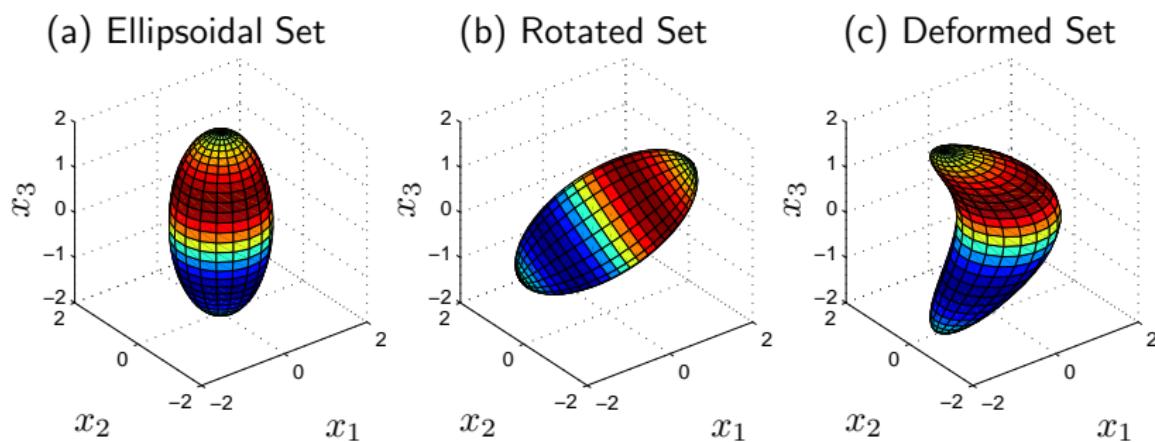
- $k$  is the *signed curvature*.

Formula in terms of  $t$ :

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



# Mappings



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

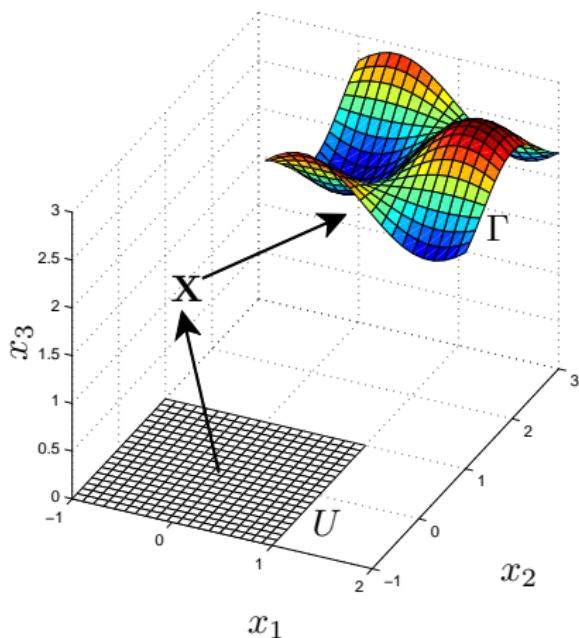
# Parametric Representation of a Surface

- 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  $\mathbf{X} : U \rightarrow \mathbb{R}^3$  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

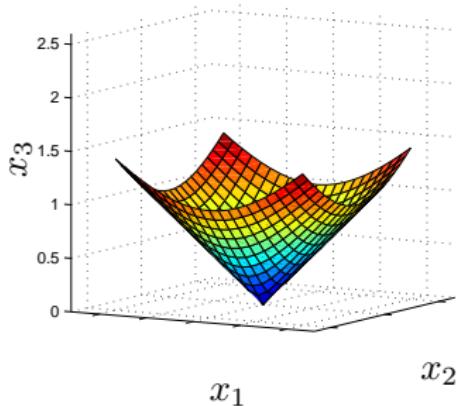
$$\mathbf{x} = \mathbf{X}(s_1, s_2).$$

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

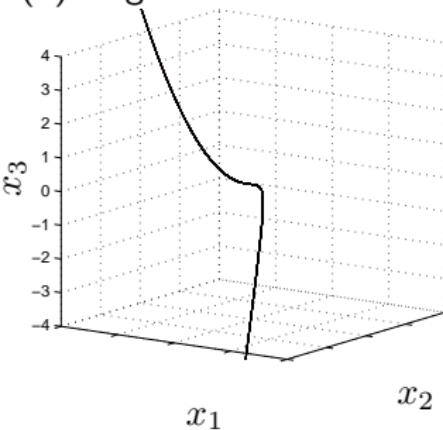


# Basic Assumptions

(a) Non-smooth Surface

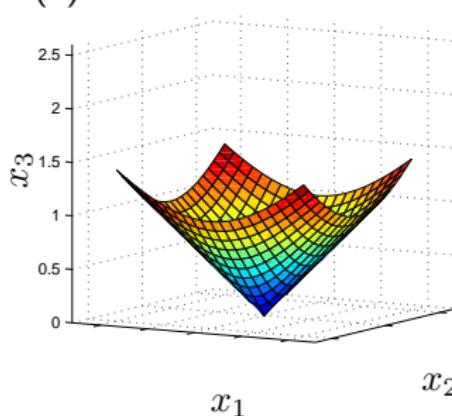


(b) Degenerate Surface

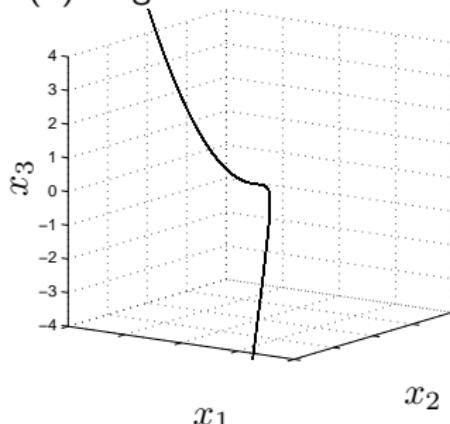


# Basic Assumptions

(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  $3 \times 2$  Jacobian matrix

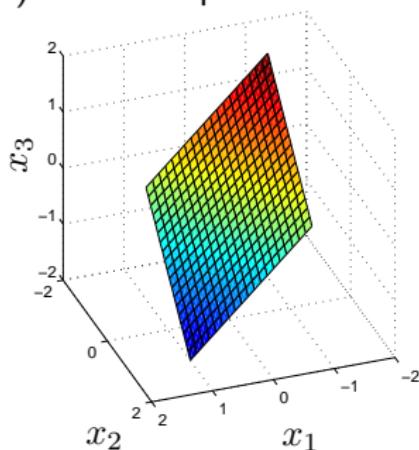
$$J = [\partial_{s_1} \mathbf{X}, \partial_{s_2} \mathbf{X}] = \nabla_s \mathbf{X}$$

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

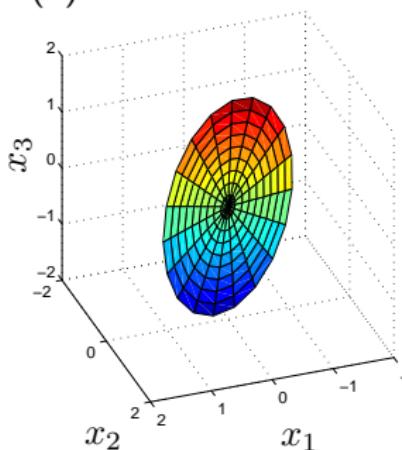
$$\mathbf{X}(s_1, s_2) = (s_1 + s_2, (s_1 + s_2)^2, (s_1 + s_2)^3)^\dagger$$

# Parameterization of a Plane

(a) Cartesian parameterization



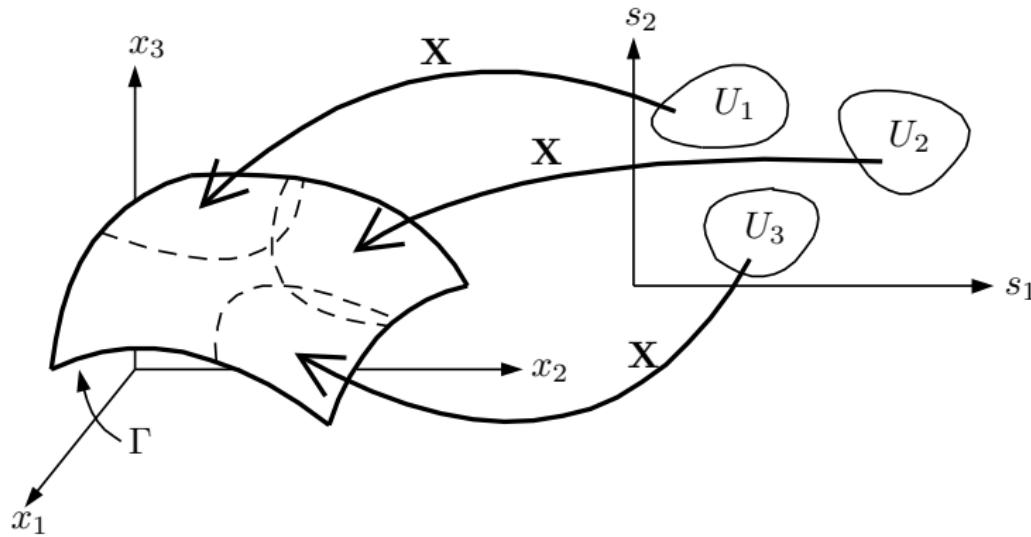
(b) Polar coordinates



- 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  $U = (0, \infty) \times (0, 2\pi)$ .

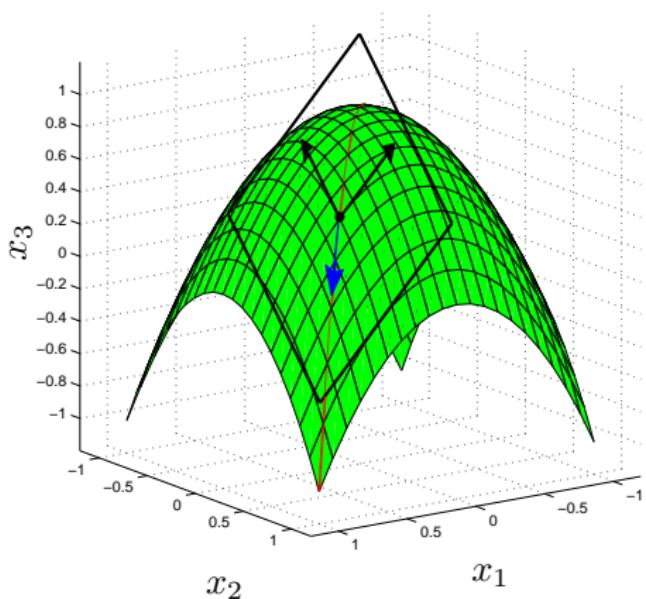
# Regular Surface; Local Charts

- 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:

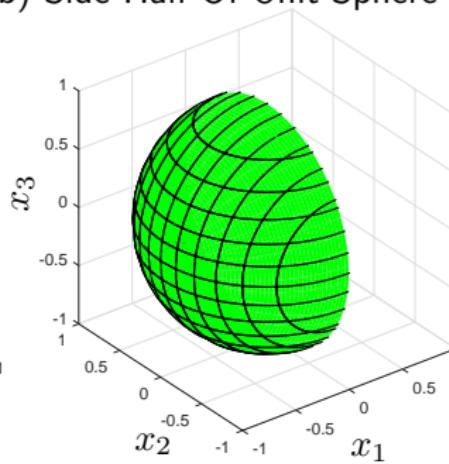
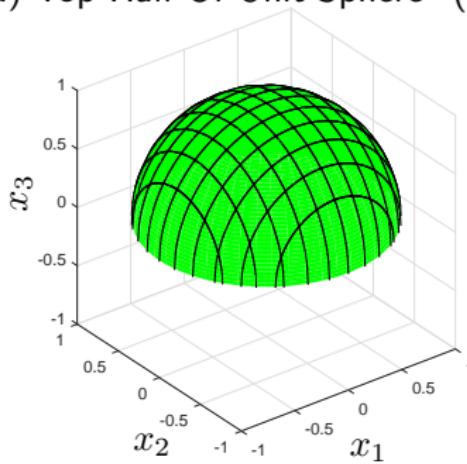
- Let  $T_{\mathbf{x}}(\Gamma)$  denote the tangent plane of the surface  $\Gamma$  at the point  $\mathbf{x}$ .

# 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:

$$g_{11} = \partial_{s_1} \mathbf{X} \cdot \partial_{s_1} \mathbf{X} = 1 + (N_1/N_3)^2,$$

$$g_{12} = \partial_{s_1} \mathbf{X} \cdot \partial_{s_2} \mathbf{X} = g_{21} = (N_1/N_3)(N_2/N_3),$$

$$g_{22} = \partial_{s_2} \mathbf{X} \cdot \partial_{s_2} \mathbf{X} = 1 + (N_2/N_3)^2,$$

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  $U = \{(s_1, s_2)^\dagger \in \mathbb{R}^2 : s_1^2 + s_2^2 < 1\}$ .

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  $(s_1^2 + s_2^2) \rightarrow 1$ .

# Metric Tensor

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

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

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  $\delta_{ij}$  is the “Kronecker delta”:

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

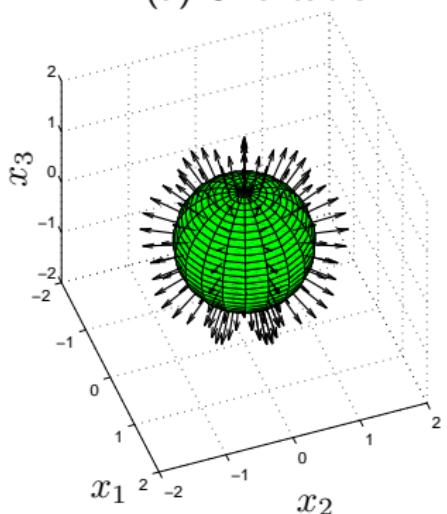
# Normal Vector

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

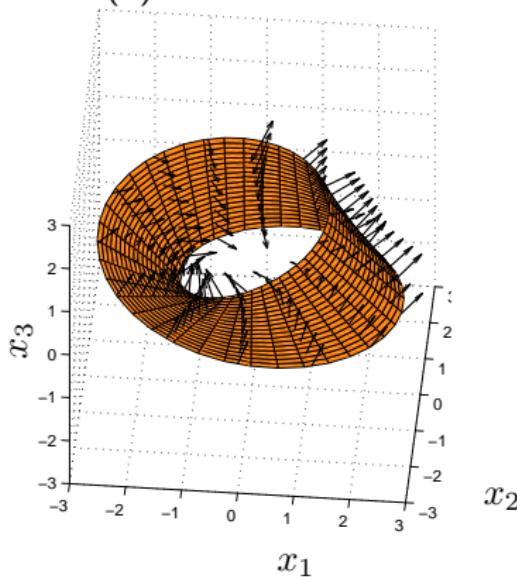
$$\nu(\mathbf{s}) = \nu(s_1, s_2) = \frac{\partial_{s_1} \mathbf{X}(\mathbf{s}) \times \partial_{s_2} \mathbf{X}(\mathbf{s})}{|\partial_{s_1} \mathbf{X}(\mathbf{s}) \times \partial_{s_2} \mathbf{X}(\mathbf{s})|} = \frac{\partial_{s_1} \mathbf{X}(\mathbf{s}) \times \partial_{s_2} \mathbf{X}(\mathbf{s})}{\sqrt{\det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

- 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  $\Gamma$ , 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.

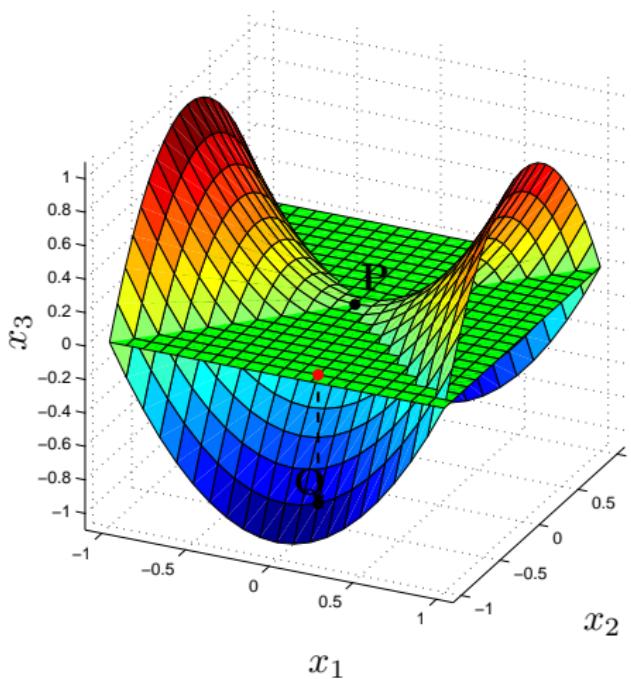
- Standard change of variable formula for surface integrals.

# Deviating From The Tangent Plane

- Curved surface  $\Gamma$ .
- 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:  $\text{dist}(Q, T_P(\Gamma)) =$

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

where  $\boldsymbol{\nu}$  is the normal vector of  $\Gamma$  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  $2 \times 2$  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:

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

# Shape Operator and Curvature

- Define the  $2 \times 2$  matrix  $S := -hg^{-1}$ .
- This is the **shape operator** of the surface.
- The eigenvalues of  $S$  are the **principle curvatures**  $\kappa_1$  and  $\kappa_2$ .
- $\kappa_1$  and  $\kappa_2$  do *not* depend on the parameterization.

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Definitions of Curvature:

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

Formulas:

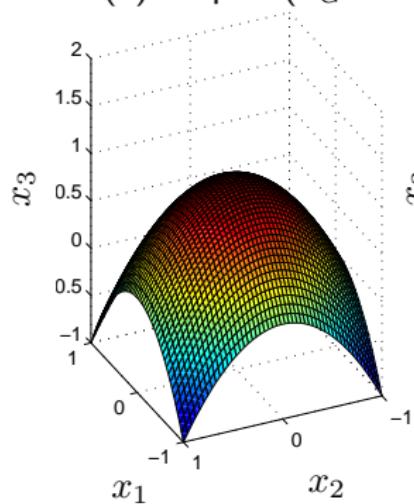
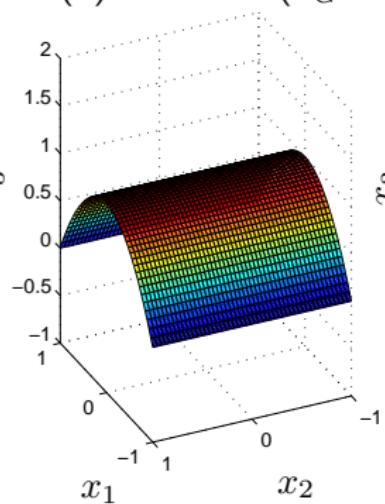
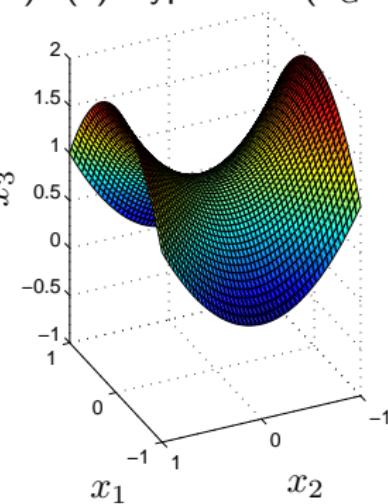
- Summed curvature:

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

- Gauss curvature:

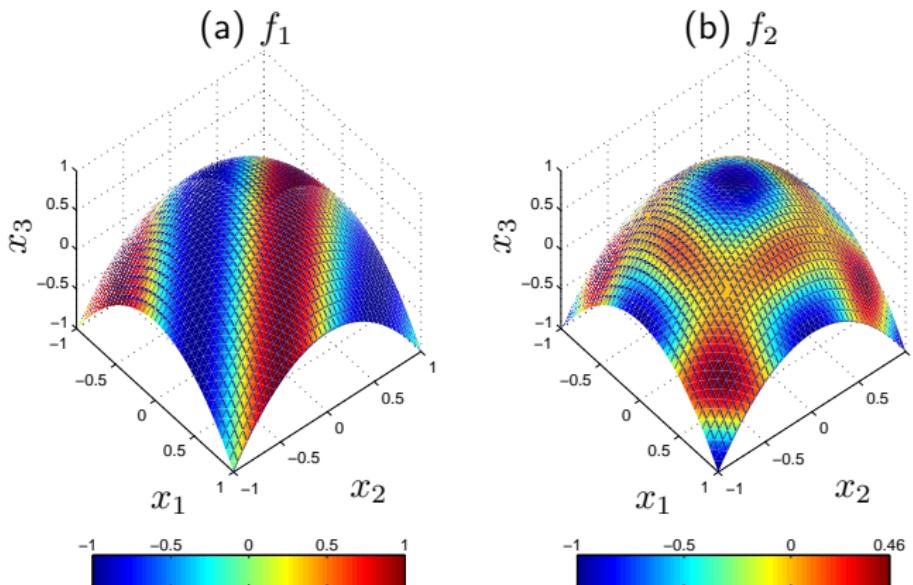
$$\kappa_G := \det S = \frac{\det(-h)}{\det g} = \frac{\det h}{\det g}$$

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

# Tangent Vector Fields

- A **tangential vector field**  $\mathbf{v} : \Gamma \rightarrow \mathbb{R}^3$  is such that  $\mathbf{v}(\mathbf{x}) \in T_{\mathbf{x}}(\Gamma)$  for all  $\mathbf{x}$  in  $\Gamma$ .
- 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.

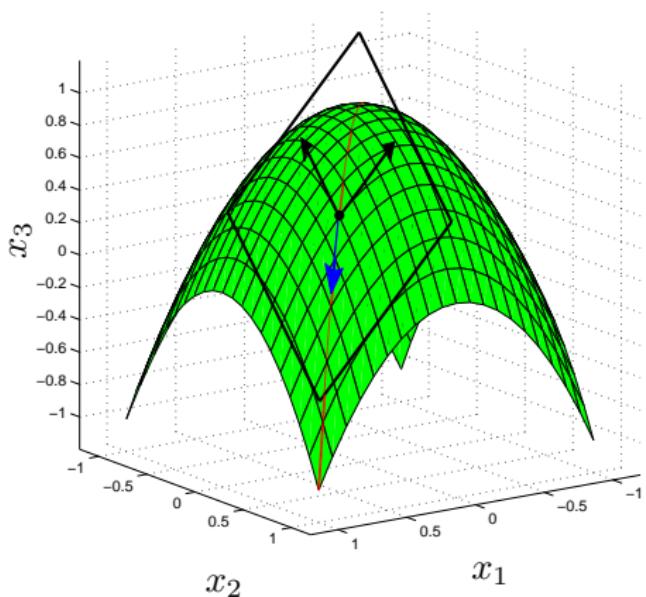
- We say  $\mathbf{v}$  is smooth, i.f.f.  $q_1, q_2$  are smooth.

# Tangential Directional Derivative

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

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

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



# Explicit Calculation

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

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Therefore, the chain rule gives

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

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

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

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

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

# Surface Gradient Operator

Hence, we obtain

$$\begin{aligned}\frac{d}{dt} \omega(\boldsymbol{\alpha}(t)) \Big|_{t=0} &= \nabla \tilde{\omega} g^{-1} (\nabla_s \mathbf{X})^\dagger \boldsymbol{\alpha}'(t) \Big|_{t=0} \\ \Rightarrow D_{\mathbf{v}} \omega(P) &= \underbrace{\nabla \tilde{\omega} g^{-1} (\nabla_s \mathbf{X})^\dagger}_{1 \times 3 \text{ row vector}} \cdot \mathbf{v}.\end{aligned}$$

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In general,

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

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

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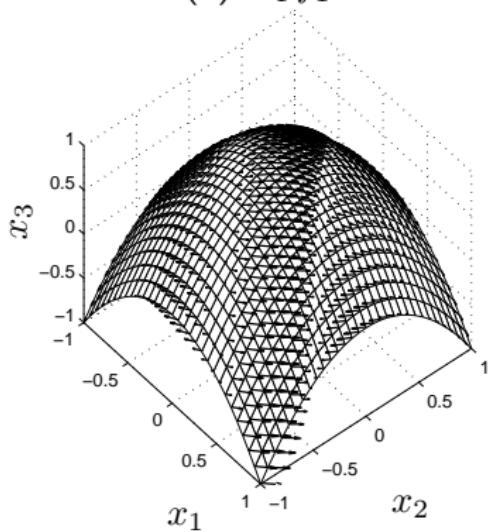
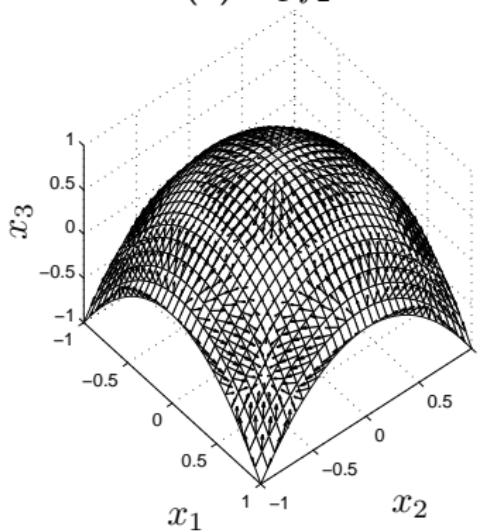
evaluated at  $\mathbf{s}$  with  $P = \mathbf{X}(\mathbf{s})$ .

- Denote the **surface gradient** of  $\omega$  at  $P$  in  $\Gamma$  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,

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

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

# Surface Gradient Example

(a)  $\nabla_{\Gamma} f_1$ (b)  $\nabla_{\Gamma} f_2$ 

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

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

# Other Surface Operators; Curvatures

## Surface Operators:

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

## Alternate curvature formulas:

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

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

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

# Integration by Parts on Surfaces

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

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

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

Another integration by parts formula:

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

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

# Shape Functionals

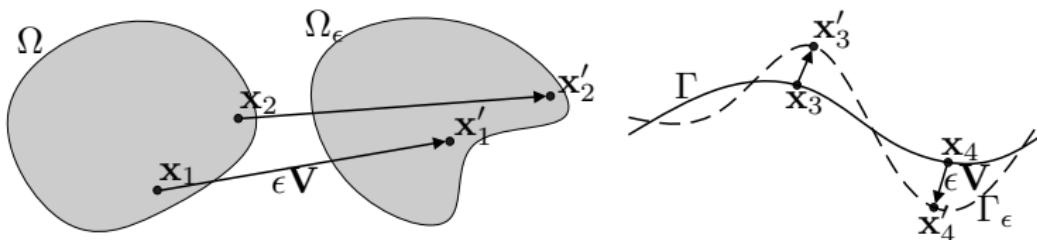
- Recall shape functionals:

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

- 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:

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

where  $\Omega_\epsilon = \Phi_\epsilon(\Omega)$ .

- Mapping an embedded surface:

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

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

# Perturbing Functions

- **Material derivative:**

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

- Extend  $f$  to all of  $\Omega_{\text{ALL}}$  such that

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

- Differentiate:

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

- **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  $\Omega$ :

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

- Perturbing functions  $g$  defined on  $\Gamma$ :

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

Other examples:

- Local perturbation of  $\Gamma$ :

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

- Perturb the normal vector:

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

- Perturb the summed curvature:

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

# 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:

$$\delta \mathcal{E}(\Omega) \cdot \mathbf{V} \equiv \delta \mathcal{E}(\Omega; \mathbf{V}) := \frac{d}{d\epsilon} \mathcal{E}_\epsilon \Big|_{\epsilon=0^+},$$

$$\delta \mathcal{J}(\Gamma) \cdot \mathbf{V} \equiv \delta \mathcal{J}(\Gamma; \mathbf{V}) := \frac{d}{d\epsilon} \mathcal{J}_\epsilon \Big|_{\epsilon=0^+},$$

$$\delta \mathcal{B}(\Gamma) \cdot \mathbf{V} \equiv \delta \mathcal{B}(\Gamma; \mathbf{V}) := \frac{d}{d\epsilon} \mathcal{B}_\epsilon \Big|_{\epsilon=0^+}.$$

# Perturbing Functionals

\*divergence thm

recall intro. example

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

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

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

# Structure Theorem

- Hadamard-Zolésio structure theorem.
- $\Omega$  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

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

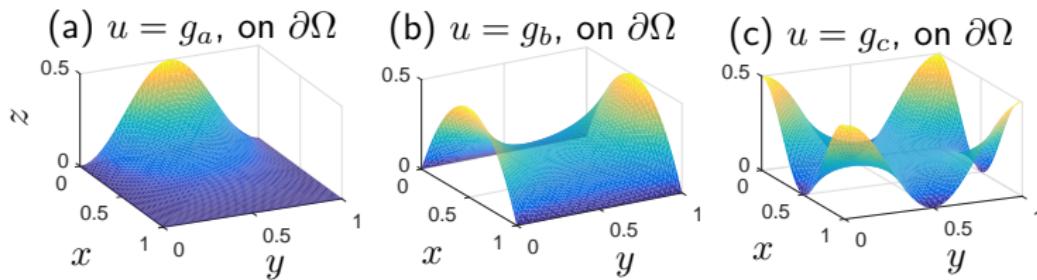
for some function  $\eta$  in  $L^1(\partial\Omega)$ .

- 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



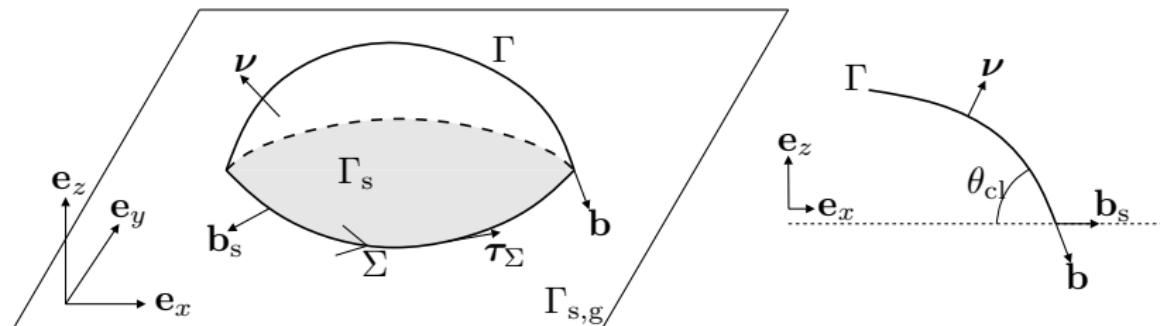
- Let  $\Gamma$  be a surface with boundary  $\partial\Gamma \equiv \Sigma$ .
- Perimeter functional:  $\mathcal{J}(\Gamma) = \int_{\Gamma} 1 dS$ .
- What is the first order optimality condition?
- Apply shape perturbation formula with  $f = 1$ :

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

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

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

# Surface Tension



- Let  $\gamma$  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”:

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

where  $\mathbf{V}$  is a perturbation of the surface  $\Gamma$ . Note:  $\mathbf{b} = \tau_{\Sigma} \times \nu$ .

- $\delta \mathcal{J}(\Gamma; \mathbf{V})$  is the relative force exerted by surface tension against deforming the surface by  $\mathbf{V}$ .
- Integral over  $\Sigma$  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  $b : \mathbb{V}(\Gamma) \times \mathbb{V}(\Gamma) \rightarrow \mathbb{R}$  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

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

# $L^2$ -Gradient Descent

## Discretize time:

- Start with an initial domain  $\Gamma^0$ .
- **FOR**  $i = 0, 1, 2, \dots$ , 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:

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

where  $\mathbf{X}^i$  is a parameterization of  $\Gamma^i$ , and  $\Delta t$  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  $\Delta t$  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  $\Gamma$  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

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

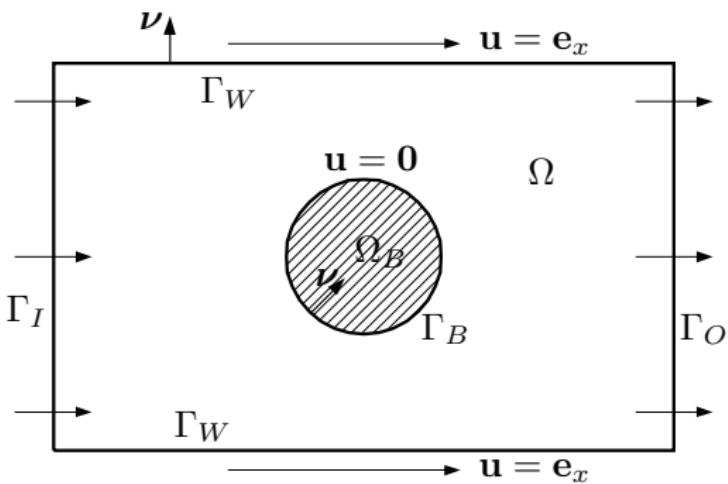
- Therefore,  $\mathbf{V}(t, \mathbf{x}) = -\kappa(t, \mathbf{x}) \boldsymbol{\nu}(t, \mathbf{x})$ , for all  $\mathbf{x} \in \Gamma(t)$ .
- The surface  $\Gamma(t)$  moves with normal velocity:

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

- 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:

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

- Cost functional:  $\mathcal{J}(\Omega) = -\mathbf{e}_x \cdot \int_{\Gamma_B} \boldsymbol{\sigma}(\mathbf{u}, p) \nu$  (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

Define  $\varphi := \mathbf{u} - \mathbf{e}_x$ :  $\Rightarrow \nabla \cdot \varphi = 0$ , in  $\Omega$ ,

$$\varphi = -\mathbf{e}_x, \text{ on } \Gamma_B,$$

$$\varphi = \mathbf{0}, \text{ on } \Gamma_I \cup \Gamma_W.$$

- Manipulate the cost:

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

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

# Differentiate The Cost

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

Apply shape perturbation formula:

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

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

# Differentiate The PDE

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

# Differentiate The PDE

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

$$\begin{aligned}\text{int. by parts } = & \int_{\Omega} \left[ (\mathbf{u}' \cdot \nabla) \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u}' - \nabla \cdot \boldsymbol{\sigma}' \right] \cdot \boldsymbol{\varphi} + \int_{\partial\Omega} \boldsymbol{\sigma}' \boldsymbol{\nu} \cdot \boldsymbol{\varphi} \\ & + \int_{\Omega} [(\mathbf{u} \cdot \nabla) \mathbf{u} - \nabla \cdot \boldsymbol{\sigma}] \cdot \mathbf{u}' + \int_{\partial\Omega} \boldsymbol{\sigma} \boldsymbol{\nu} \cdot \mathbf{u}' + \\ & + \int_{\Gamma_B} (\mathbf{V} \cdot \boldsymbol{\nu}) [(\mathbf{u} \cdot \nabla) \mathbf{u}] \cdot \boldsymbol{\varphi} + \frac{2}{\text{Re}} \int_{\Gamma_B} (\mathbf{V} \cdot \boldsymbol{\nu}) |D(\mathbf{u})|^2\end{aligned}$$

$$(\mathbf{u} \cdot \nabla) \mathbf{u} - \nabla \cdot \boldsymbol{\sigma} = \mathbf{0}, \text{ in } \Omega,$$

$$(\mathbf{u}' \cdot \nabla) \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u}' - \nabla \cdot \boldsymbol{\sigma}' = \mathbf{0}, \text{ in } \Omega,$$

$$\nabla \cdot \mathbf{u} = 0, \text{ in } \Omega,$$

$$\nabla \cdot \mathbf{u}' = 0, \text{ in } \Omega,$$

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

$$\mathbf{u}' = ??, \text{ on } \Gamma_B,$$

$$\mathbf{u} = \mathbf{e}_x, \text{ on } \Gamma_I \cup \Gamma_W,$$

$$\mathbf{u}' = \mathbf{0}, \text{ on } \Gamma_I \cup \Gamma_W,$$

$$\boldsymbol{\sigma} \boldsymbol{\nu} = \mathbf{0}, \text{ on } \Gamma_O.$$

$$\boldsymbol{\sigma}' \boldsymbol{\nu} = \mathbf{0}, \text{ on } \Gamma_O.$$

# Use The Adjoint Variable

- The shape perturbation reduces to

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

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

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

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

# Simplify

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

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

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

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

- This satisfies the structure theorem.
- $\eta$  is sometimes called the **shape gradient**.

# Shape Gradient Descent

- Start with an initial domain  $\Gamma_B^i$ .
- **FOR**  $i = 0, 1, 2, \dots$ , do the following.
- Solve for  $(\mathbf{u}, p)$  and  $(\mathbf{r}, \pi)$  on  $\Omega^i$ .
- Evaluate  $\eta^i$ .
- 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  $\Gamma_B^{i+1}$  (**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

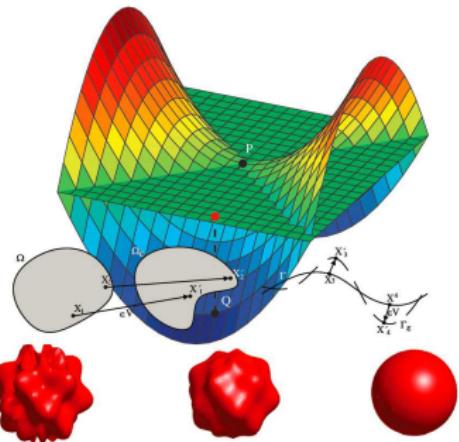
- Moving interfaces often involve curvature.
- Can be understood in the context of shape differentiation.
- Shape gradients necessary for *shape optimization*.

**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.

## The Shapes of Things

*A Practical Guide to Differential Geometry and the Shape Derivative*



Shawn W. Walker



# 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.

Special thanks to



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