Lecture 6: Shape derivatives of PDE constrained functionals.

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Recap

Given a Lipschitz domain Ω, we parameterize deformations of Ω by a continuous vector field $\boldsymbol{\theta}$:

$$\Omega_{\boldsymbol{\theta}} := (I + \boldsymbol{\theta})\Omega = \{x + \boldsymbol{\theta}(x) \,|\, x \in \Omega\}$$

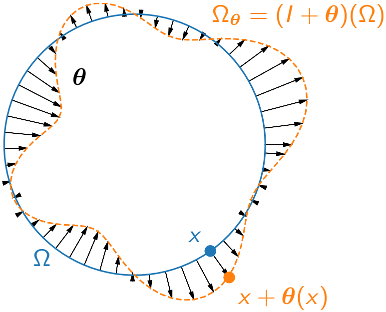


Figure: Deformation of a domain Ω with the method of Hadamard. A small vector field $\boldsymbol{\theta}$ is used to deform Ω into $\Omega_{\boldsymbol{\theta}} = (I + \boldsymbol{\theta})\Omega$.

Recap

Let $J(\Omega)$ denote a shape functional arising e.g. in a shape optimization problem

$$\min_{\Omega} \; J(\Omega).$$

Definition 1

A shape functional $J(\Omega)$ is said shape differentiable if the mapping

$$\begin{array}{rcl} W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d) & \longrightarrow & \mathbb{R} \\ \boldsymbol{\theta} & \longmapsto & J(\Omega_{\boldsymbol{\theta}}) \end{array}$$

is Fréchet differentiable at $\boldsymbol{\theta} = 0$, *i.e.* if there exists a continuous linear form

$$\mathrm{D}J(\Omega) \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)^*$$

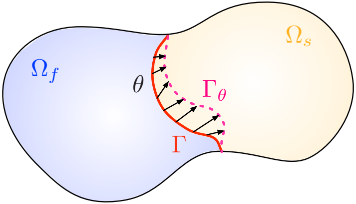
such that the following asymptotics holds true:

$$J(\Omega_{\boldsymbol{\theta}}) = J(\Omega) + \mathrm{D}J(\Omega)(\boldsymbol{\theta}) + o(\boldsymbol{\theta}), \qquad \text{where} \quad \frac{|o(\boldsymbol{\theta})|}{||\boldsymbol{\theta}||_{W^{1,\infty}(\mathbb{R}^d,\mathbb{R}^d)}} \xrightarrow{\boldsymbol{\theta}\to 0} 0.$$

The **linear form** $\mathrm{D}J(\Omega)$ is called the shape derivative of J on the domain Ω.

The boundary variation method of Hadamard

$$\min_{\Gamma} \; J(\Gamma)$$



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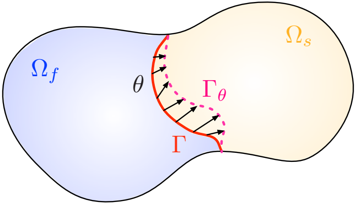

$$\Gamma_{\boldsymbol{\theta}} = (I + \boldsymbol{\theta})\Gamma, \text{ with } \boldsymbol{\theta} \in W_0^{1,\infty}(D, \mathbb{R}^d), \;\; ||\boldsymbol{\theta}||_{W^{1,\infty}(\mathbb{R}^d,\mathbb{R}^d)} < 1.$$

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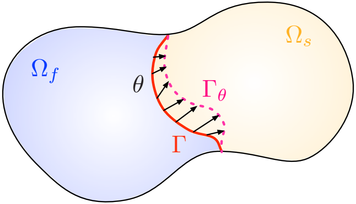

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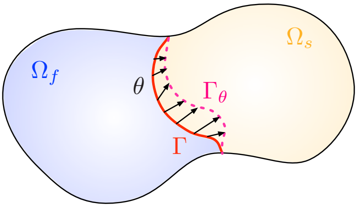

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Under suitable regularity assumptions, Hadamard structure theorem holds:

$$\frac{\mathrm{d}J}{\mathrm{d}\boldsymbol{\theta}}(\Gamma)(\boldsymbol{\theta}) = \int_{\Gamma} v_J(\Gamma)\, \boldsymbol{\theta} \cdot \boldsymbol{n} \mathrm{d}\sigma$$

for some $v_J(\Gamma) \in L^1(\Gamma)$.

The boundary variation method of Hadamard

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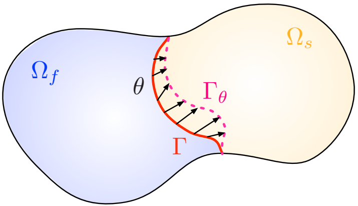

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for some $v_J(\Gamma) \in L^1(\Gamma)$.

If $\boldsymbol{\theta} \cdot \boldsymbol{n} = -v_J(\Gamma)$ on Γ, then $J(\Gamma_{\boldsymbol{\theta}}) = J(\Gamma) - t \int_\Gamma |v_J(\Gamma)|^2 \mathrm{d}\sigma + o(t) < J(\Gamma)$; $\boldsymbol{\theta}$ is a descent direction.

Proposition 1

Let Ω be a bounded open set of $\mathbb{R}^d$. For any $f \in W^{1,1}(\mathbb{R}^d)$, the functional $J(\Omega)$ defined by

$$J(\Omega) := \int_\Omega f(x)\mathrm{d}x$$

is shape differentiable, and it holds

$$\mathrm{D}J(\Omega)(\boldsymbol{\theta}) = \int_\Omega \mathrm{div}(f\boldsymbol{\theta})\mathrm{d}x = \int_\Omega (\nabla f \cdot \boldsymbol{\theta} + f\,\mathrm{div}(\boldsymbol{\theta}))\mathrm{d}x, \qquad \boldsymbol{\theta} \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d).$$

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If in addition Ω is smooth then the above formula can be rewritten as

$$\mathrm{D}J(\Omega)(\boldsymbol{\theta}) = \int_{\partial\Omega} f\,\boldsymbol{\theta} \cdot \boldsymbol{n}\mathrm{d}\sigma, \qquad \boldsymbol{\theta} \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d).$$

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Surface form of the shape derivative.

Proposition 2

Let Γ *be a smooth codimension one surface of* $\mathbb{R}^d$ *with boundary* $\partial\Gamma$. *For any* $f \in W^{2,1}(\mathbb{R}^d)$, *the functional* $J(\Gamma)$ *defined by*

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where $\boldsymbol{\tau}$ denotes the outward normal to $\partial\Gamma$ tangent to Γ.

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$\kappa = \mathrm{div}(\boldsymbol{n})$ is the mean curvature field of Γ.

Outline

1. A model problem
2. Eulerian and Lagrangian derivatives
3. The adjoint state
4. Volume form and surface form of the shape derivative
5. Shape derivatives of arbitrary functionals

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A model problem

Consider the shape optimization problem

$$\min_{\Omega} \int_{\Omega} j(u)\mathrm{d}x$$

$$s.t. \begin{cases} -\Delta u = f \text{ in } \Omega, \\ u = 0 \text{ on } \Gamma_D, \\ \dfrac{\partial u}{\partial \boldsymbol{n}} = 0 \text{ on } \Gamma_N. \end{cases}$$

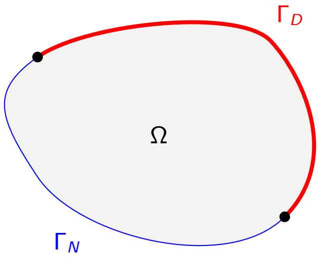

Figure: Setting for the Poisson problem.

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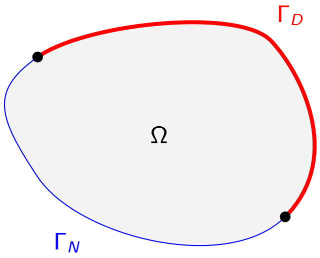

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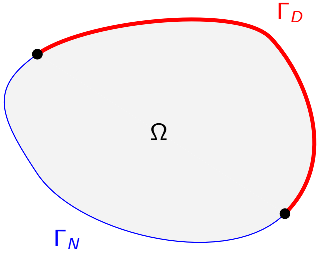

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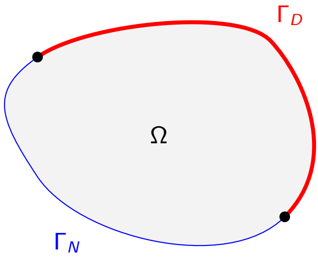

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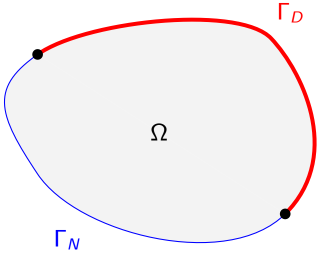

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- Let $\Gamma_{D,\boldsymbol{\theta}} := (I + \boldsymbol{\theta})\Gamma_D$, $\Gamma_{N,\boldsymbol{\theta}} = (I + \boldsymbol{\theta})\Gamma_N$ and $u_{\boldsymbol{\theta}}$ the solution to the Laplace problem on $\Omega_{\boldsymbol{\theta}}$.

A model problem

Consider the shape minimization problem

$$\min_{\boldsymbol{\theta} \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)} \int_{\Omega_{\boldsymbol{\theta}}} j(u_{\boldsymbol{\theta}}) \mathrm{d}x$$

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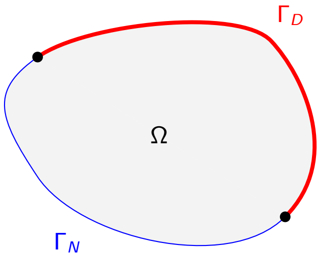

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A model problem

Our goal: find the Fréchet derivative of

$$\boldsymbol{\theta} \mapsto J(\Omega_{\boldsymbol{\theta}}, u_{\boldsymbol{\theta}}) = \int_{\Omega_{\boldsymbol{\theta}}} j(u_{\boldsymbol{\theta}})\mathrm{d}x, \qquad \boldsymbol{\theta} \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d),$$

where

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Outline

The Eulerian derivative

Naively,

$$\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}} J(\Omega_{\boldsymbol{\theta}}, u_{\boldsymbol{\theta}}) = \int_{\partial\Omega} j(u)\boldsymbol{\theta} \cdot \boldsymbol{n} \mathrm{d}\sigma + \int_{\Omega} j'(u) \left(\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}} u_{\boldsymbol{\theta}} \right) (\boldsymbol{\theta}) \mathrm{d}x \tag{1}$$

where $\boldsymbol{\theta} \mapsto \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}} u_{\boldsymbol{\theta}}$ would be the derivative of $\boldsymbol{\theta} \mapsto u_{\boldsymbol{\theta}}(x)$ with $x \in \Omega$.

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- Difficulty 2: the functions $u_{\boldsymbol{\theta}} \in H^1(\Omega_{\boldsymbol{\theta}})$ and $u \in H^1(\Omega)$ belong to different definition spaces.
- Difficulty 3: the Eulerian derivative does not always exist and eq. (1) does not make sense.

The Lagrangian derivative

Another approach: change of variable in fixed reference domain. Let

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The variational formulation of

$$\begin{cases} -\Delta u_{\boldsymbol{\theta}} = f \text{ in } \Omega_{\boldsymbol{\theta}}, \\ u_{\boldsymbol{\theta}} = 0 \text{ on } \Gamma_{D,\boldsymbol{\theta}}, \\ \dfrac{\partial u_{\boldsymbol{\theta}}}{\partial \boldsymbol{n}} = 0 \text{ on } \Gamma_{N,\boldsymbol{\theta}}. \end{cases}$$

reads find $u_{\boldsymbol{\theta}} \in V_{\boldsymbol{\theta}}$ such that

$$\int_{\Omega_{\boldsymbol{\theta}}} \nabla u_{\boldsymbol{\theta}} \cdot \nabla v \mathrm{d}x = \int_{\Omega_{\boldsymbol{\theta}}} f v \mathrm{d}x, \qquad \forall v \in V_{\boldsymbol{\theta}}.$$

The Lagrangian derivative

Another approach: change of variable in fixed reference domain. Let

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The variational formulation of

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After the change of variable $x = (I + \boldsymbol{\theta})(y)$:

$$\int_{\Omega} [(\nabla u_{\boldsymbol{\theta}}) \circ (I + \boldsymbol{\theta})] \cdot [(\nabla v) \circ (I + \boldsymbol{\theta})] \det(I + \nabla \boldsymbol{\theta}) \mathrm{d}y = \int_{\Omega} f \circ (I + \boldsymbol{\theta}) v \circ (I + \boldsymbol{\theta}) \det(I + \nabla \boldsymbol{\theta}) \mathrm{d}y.$$

Lemma 3

Let $f \in H^1(\mathbb{R}^d)$ and $\boldsymbol{f} \in H^1(\mathbb{R}^d, \mathbb{R}^d)$ be respectively scalar and vectorial functions, and $\boldsymbol{\theta} \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ with $||\boldsymbol{\theta}||_{W^{1,\infty}(\mathbb{R}^d,\mathbb{R}^d)} < 1$. It holds

$$(\nabla f) \circ (I + \boldsymbol{\theta}) = (I + \nabla\boldsymbol{\theta})^{-T} \nabla(f \circ (I + \boldsymbol{\theta}))$$
$$(\nabla \boldsymbol{f}) \circ (I + \boldsymbol{\theta}) = \nabla(\boldsymbol{f} \circ (I + \boldsymbol{\theta}))(I + \nabla\boldsymbol{\theta})^{-1}.$$

Remark 1

$\nabla f = (\partial_i f)_{1\le i\le d}$ is a row vector while $\nabla \boldsymbol{f} = (\partial_j f_i)_{1\le i,j\le d} = \begin{bmatrix}\nabla f_1^T & \cdot & \nabla f_d^T\end{bmatrix}$.

The Lagrangian derivative

$$\int_\Omega [(\nabla u_{\boldsymbol{\theta}}) \circ (I + \boldsymbol{\theta})] \cdot [\nabla v \circ (I + \boldsymbol{\theta})] \det(I + \nabla \boldsymbol{\theta}) \mathrm{d}y = \int_\Omega f \circ (I + \boldsymbol{\theta}) v \circ (I + \boldsymbol{\theta}) \det(I + \nabla \boldsymbol{\theta}) \mathrm{d}y,$$

rewrites as

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rewrites as find $u_{\boldsymbol{\theta}} \circ (I + \boldsymbol{\theta}) \in V$ such that for any $v \in V$,

$$\langle F(\boldsymbol{\theta}, u_{\boldsymbol{\theta}} \circ (I + \boldsymbol{\theta})), v \rangle_{V,V'} = 0 \tag{2}$$

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where

$$\langle F(\boldsymbol{\theta}, u), v \rangle_{V,V'} = \int_\Omega (I + \nabla \boldsymbol{\theta})^{-T} \nabla u \cdot (I + \nabla \boldsymbol{\theta})^{-T} \nabla v \det(I + \nabla \boldsymbol{\theta}) \mathrm{d}x - \int_\Omega f \circ (I + \boldsymbol{\theta}) \det(I + \nabla \boldsymbol{\theta}) \, v \mathrm{d}x.$$

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- $u_{\boldsymbol{\theta}} \circ (I+\boldsymbol{\theta})$ belongs to the fixed space V!

The Lagrangian derivative

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- $u_{\boldsymbol{\theta}} \circ (I + \boldsymbol{\theta})$ belongs to the fixed space V!
- $F : W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d) \times V \to V'$ is such that $\partial F / \partial u$ is invertible at $(0, u(\Omega))$.

The Lagrangian derivative

$$\int_\Omega [(\nabla u_{\boldsymbol\theta})\circ(I+\boldsymbol\theta)]\cdot[\nabla v\circ(I+\boldsymbol\theta)]\,\det(I+\nabla\boldsymbol\theta)\mathrm{d}y = \int_\Omega f\circ(I+\boldsymbol\theta)v\circ(I+\boldsymbol\theta)\,\det(I+\nabla\boldsymbol\theta)\mathrm{d}y,$$

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The Lagrangian derivative

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- The implicit function theorem yields the existence of $\boldsymbol{\theta}\mapsto u_{\boldsymbol{\theta}}\circ(I+\boldsymbol{\theta})$ solving eq. (2).
- Since $\boldsymbol{\theta}\mapsto F(\boldsymbol{\theta}, u)$ is Fréchet differentiable, it follows that $\boldsymbol{\theta}\mapsto u_{\boldsymbol{\theta}}\circ(I+\boldsymbol{\theta})$ is Fréchet differentiable as a mapping $W^{1,\infty}(\mathbb{R}^d,\mathbb{R}^d)\to V$.

Definition 4

The Fréchet derivative of the mapping $\boldsymbol{\theta} \mapsto u_{\boldsymbol{\theta}} \circ (I + \boldsymbol{\theta})$, $W^{1\infty}(\mathbb{R}^d, \mathbb{R}^d) \to V$ at $\boldsymbol{\theta} = 0$, is called the *Lagrangian derivative* of $u_{\boldsymbol{\theta}}$, and is denoted by $\dot{u}(\boldsymbol{\theta})$.

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$$\dot{u}(\boldsymbol{\theta})(x) = u'(\boldsymbol{\theta}) + \nabla u_{\boldsymbol{\theta}} \cdot \boldsymbol{\theta},$$

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It is safer to work with Lagrangian derivatives!

Computation of $\dot{u}$

Differentiating

$$0 = \langle F(\boldsymbol{\theta}, u), v \rangle_{V,V'} = \int_\Omega (I + \nabla\boldsymbol{\theta})^{-T} \nabla u \cdot (I + \nabla\boldsymbol{\theta})^{-T} \nabla v \det(I + \nabla\boldsymbol{\theta}) \mathrm{d}x$$
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with respect to $\boldsymbol{\theta}$ yields

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with respect to $\boldsymbol{\theta}$ yields

$$0 = \int_\Omega (I - \nabla\boldsymbol{\theta} - \nabla\boldsymbol{\theta}^T + \mathrm{div}(\boldsymbol{\theta})I)\nabla\dot{u} \cdot \nabla v\mathrm{d}x - \int_\Omega (\nabla f \cdot \boldsymbol{\theta} + \mathrm{div}(\boldsymbol{\theta})f)v\mathrm{d}x$$

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i.e. find $\dot{u}(\boldsymbol{\theta}) \in V$ such that

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Remark 3

When differentiating $0 = \int_\Omega \nabla u \cdot \nabla v \mathrm{d}x - \int_\Omega f v \mathrm{d}x$:

- the shape differentiation of ∇f yields a term $-\nabla\boldsymbol{\theta}^T \nabla f$, of f a term $\nabla f \cdot \boldsymbol{\theta}$;

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This is a well-posed variational formulation which gives the value of $\dot{u}(\boldsymbol{\theta})$ for any $\boldsymbol{\theta} \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$.

A first expression of the shape derivative

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$$\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}} J(\Omega_{\boldsymbol{\theta}}, u_{\boldsymbol{\theta}})\mathrm{d}x = \int_{\Omega} (j'(u)\dot{u}(\boldsymbol{\theta}) + j(u)\mathrm{div}(\boldsymbol{\theta}))\mathrm{d}x.$$

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Although explicit, this formula is not satisfactory because

- $\dot{u}(\boldsymbol{\theta})$ is defined as the solution of a PDE depending on every value of $\boldsymbol{\theta} \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$.

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Although explicit, this formula is not satisfactory because

- $\dot{u}(\boldsymbol{\theta})$ is defined as the solution of a PDE depending on every value of $\boldsymbol{\theta} \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$.
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The classical trick is to introduce an adjoint state.

Outline

1. A model problem
2. Eulerian and Lagrangian derivatives
3. The adjoint state
4. Volume form and surface form of the shape derivative
5. Shape derivatives of arbitrary functionals

The adjoint state

Suppose that we want to compute the derivative of some function

$$J(\boldsymbol{\theta}) = f(u(\boldsymbol{\theta})) \qquad s.t. \qquad A(\boldsymbol{\theta})u(\boldsymbol{\theta}) = f.$$

for some matrix $A(\boldsymbol{\theta})$.

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In our setting,

$$\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}} J(\Omega_{\boldsymbol{\theta}}, u_{\boldsymbol{\theta}})\mathrm{d}x = \int_\Omega (j'(u)\dot{u}(\boldsymbol{\theta}) + j(u)\mathrm{div}(\boldsymbol{\theta}))\mathrm{d}x.$$

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$$\text{Find } p \in V \text{ such that } \forall v \in V,\ \int_\Omega \nabla p \cdot \nabla v \mathrm{d}x = \int_\Omega j'(u) v \mathrm{d}x.$$

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Proposition 3

Assume $\Omega \subset D$ *is a Lipschitz bounded open set and* $f \in H^1(\mathbb{R}^d)$*. The functional* $J(\Omega, u(\Omega)) = \int_\Omega j(u)\mathrm{d}x$ *is shape differentiable and the shape derivative reads*

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- eq. (3) is called the **volume** form of the shape derivative; it is not yet written in the form of a boundary integral depending only on $\boldsymbol{\theta} \cdot \boldsymbol{n}$.

Outline

Surface expression of the shape derivative

To obtain the surface expression, we do an integration by parts:

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$$= \int_\Omega \Lambda\cdot\boldsymbol{\theta}\mathrm{d}x + \int_{\partial\Omega} (j(u)\boldsymbol{\theta}\cdot\boldsymbol{n} + (\boldsymbol{n}\cdot\nabla u)\boldsymbol{\theta}\cdot\nabla p + (\boldsymbol{n}\cdot\nabla p)(\boldsymbol{\theta}\cdot\nabla u) - \nabla u\cdot\nabla p(\boldsymbol{\theta}\cdot\boldsymbol{n}) + fp\boldsymbol{\theta}\cdot\boldsymbol{n})\mathrm{d}\sigma$$

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- Warning, the integration by parts requires u and p to be of H^2 regularity. This is wrong in the vicinity of $\Gamma_D \cap \Gamma_N$ or if Ω has corners.

Proposition 4

Assume Ω is smooth and $f \in H^1(\mathbb{R}^d)$. If $\boldsymbol{\theta} = 0$ on a neighborhood of $\Gamma_D \cap \Gamma_N$, then the shape derivative of $J(\Omega, u(\Omega))$ given by eq. (3) *rewrites as a boundary integral involving only the normal trace component $\boldsymbol{\theta} \cdot \boldsymbol{n}$ of $\boldsymbol{\theta}$:*

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- eq. (4) is called the "surface expression" of the shape derivative.

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- eq. (4) is called the "surface expression" of the shape derivative.
- A descent direction is given by

$$\boldsymbol{\theta} \cdot \boldsymbol{n} = -t \left(j(u) + fp + 2 \frac{\partial u}{\partial \boldsymbol{n}} \frac{\partial p}{\partial \boldsymbol{n}} - \nabla u \cdot \nabla p \right)$$

Self-adjoint functionals

- If $j(u) = \int_\Omega f u \mathrm{d}x$ (the compliance), then p is solution to

$$\text{Find } p \in V \text{ such that } \forall v \in V, \int_\Omega \nabla p \cdot \nabla v \mathrm{d}x = \int_\Omega f v \mathrm{d}x,$$

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Self-adjoint functionals

Consider the **compliance** minimization problem

$$\min_{\Omega} \int_{\Gamma} g u \, \mathrm{d}\sigma$$

$$s.t. \begin{cases} -\Delta u = 0 \text{ in } \Omega, \\ \dfrac{\partial u}{\partial \boldsymbol{n}} = 0 \text{ on } \Gamma_D, \\ \dfrac{\partial u}{\partial \boldsymbol{n}} = g \text{ on } \Gamma_N, \\ \dfrac{\partial u}{\partial \boldsymbol{n}} = 0 \text{ on } \Gamma. \end{cases}$$

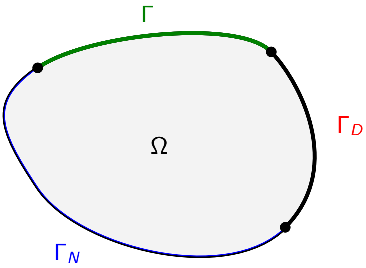

Figure: Setting for the Poisson problem.

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$$s.t. \begin{cases} -\Delta u = 0 \text{ in } \Omega, \\ \dfrac{\partial u}{\partial \boldsymbol{n}} = 0 \text{ on } \Gamma_D, \\ \dfrac{\partial u}{\partial \boldsymbol{n}} = g \text{ on } \Gamma_N, \\ \dfrac{\partial u}{\partial \boldsymbol{n}} = 0 \text{ on } \Gamma. \end{cases}$$

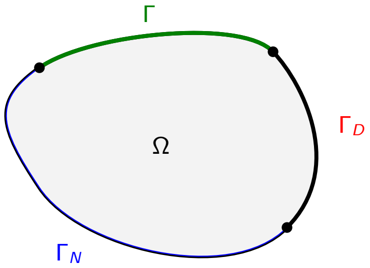

Figure: Setting for the Poisson problem.

We assume that Γ_D and Γ_N are fixed ($\boldsymbol{\theta} = 0$ on $\Gamma_D \cup \Gamma_N$).

Self-adjoint functionals

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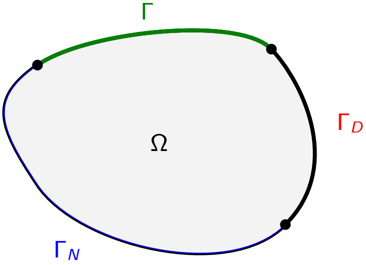

Figure: Setting for the Poisson problem.

We assume that Γ_D and Γ_N are fixed ($\boldsymbol{\theta} = 0$ on $\Gamma_D \cup \Gamma_N$).

- We still have $p = u$ and the same computation yields

$$\left.\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}}\right|_{\boldsymbol{\theta}=0} [J(\Omega_{\boldsymbol{\theta}}, u(\Omega_{\boldsymbol{\theta}}))](\boldsymbol{\theta}) = -\int_{\Gamma} |\nabla u|^2 (\boldsymbol{\theta} \cdot \boldsymbol{n}) \mathrm{d}\sigma.$$

- It is always advantageous to take $\boldsymbol{\theta} = \boldsymbol{n}$ (e.g. to add matter) to reduce the compliance.

Exercise

Compute the shape derivative of the compliance for the linear elasticity system.

$$\begin{cases} -\mathrm{div}(Ae(\boldsymbol{u})) = \boldsymbol{f} \text{ in } \Omega \\ \boldsymbol{u} = 0 \text{ on } \Gamma_D \\ Ae(\boldsymbol{u}) \cdot \boldsymbol{n} = \boldsymbol{g} \text{ on } \Gamma_N \\ Ae(\boldsymbol{u}) \cdot \boldsymbol{n} = 0 \text{ on } \Gamma \end{cases}$$

with Γ being the optimized boundary and

$$Ae(\boldsymbol{u}) = 2\mu e(\boldsymbol{u}) + \lambda \mathrm{Tr}(e(\boldsymbol{u})) \text{ with } e(\boldsymbol{u}) = \frac{\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T}{2}.$$

$$J(\Omega, \boldsymbol{u}) = \int_\Omega f \boldsymbol{u} \mathrm{d}x + \int_{\partial\Omega} \boldsymbol{g} \cdot \boldsymbol{u} \mathrm{d}\sigma$$

Outline

1. A model problem
2. Eulerian and Lagrangian derivatives
3. The adjoint state
4. Volume form and surface form of the shape derivative
5. Shape derivatives of arbitrary functionals

Shape derivatives of arbitrary functionals

In a practical implementation, for the computation of the shape derivative $\mathrm{D}J(\Omega, u(\Omega))(\boldsymbol{\theta})$, one needs:

- to specify $J(\Omega, u(\Omega))$, which requires to solve a PDE for $u(\Omega)$, e.g.

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$$\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}}[J(\Omega_{\boldsymbol{\theta}}, u_{\boldsymbol{\theta}})](\boldsymbol{\theta}) = \int_\Omega j(u)\mathrm{div}(\boldsymbol{\theta})\mathrm{d}x + \int_\Omega [(\nabla\boldsymbol{\theta} + \nabla\boldsymbol{\theta}^T - \mathrm{div}(\boldsymbol{\theta})I)\nabla u \cdot \nabla p + p\mathrm{div}(f\boldsymbol{\theta})]\mathrm{d}x,$$

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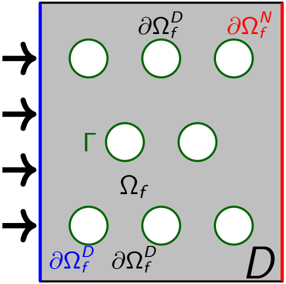
The derivation depends a priori on the form of the shape functional. We now present a procedure which works for arbitrary shape functionals.

Shape derivatives for laminar flows



Let us consider the Stokes equations:

$$\begin{cases} -\mathrm{div}(\sigma_f(\boldsymbol{v}, p)) = \boldsymbol{f}_f \text{ in } \Omega_f, \\ \boldsymbol{v} = \boldsymbol{v}_0 \text{ on } \partial\Omega_{f,D} \\ \sigma_f(\boldsymbol{v}, p) \cdot \boldsymbol{n} = 0 \text{ on } \partial\Omega_{f,N} \\ \boldsymbol{v} = 0 \text{ on } \Gamma, \\ \sigma_f(\boldsymbol{v}, p) = \nu(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T) - pI. \end{cases}$$

We want to compute the shape derivative of an arbitrary functional of the form

$$J(\Omega_f, \boldsymbol{v}(\Omega_f), p(\Omega_f)).$$

The trick: reexpress everything in terms of $\boldsymbol{v}(\Omega_{f,\boldsymbol{\theta}}) \circ (I + \boldsymbol{\theta})$ and $p(\Omega_{f,\boldsymbol{\theta}}) \circ (I + \boldsymbol{\theta})$.

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Introduce the modified functional

$$\mathfrak{J}(\boldsymbol{\theta}, \hat{\boldsymbol{v}}, \hat{p}) := J(\Omega_{f,\boldsymbol{\theta}}, \hat{\boldsymbol{v}} \circ (I+\boldsymbol{\theta})^{-1}, \hat{p} \circ (I+\boldsymbol{\theta})^{-1}),$$
$$\boldsymbol{\theta} \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d), \hat{\boldsymbol{v}} \in H^1(\Omega_f, \mathbb{R}^d), \hat{p} \in L^2(\Omega_f).$$

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Then by construction,

$$J(\Omega_{f,\boldsymbol{\theta}}, \boldsymbol{v}(\Omega_{f,\boldsymbol{\theta}}), p(\Omega_{f,\boldsymbol{\theta}})) = \mathfrak{J}(\boldsymbol{\theta}, \boldsymbol{v}(\Omega_{f,\boldsymbol{\theta}}) \circ (I + \boldsymbol{\theta}), p(\Omega_{f,\boldsymbol{\theta}}) \circ (I + \boldsymbol{\theta})).$$

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- The functional $\mathfrak{J}$ is defined on fixed spaces
- It brings naturally into play the Lagrangian derivatives

The chain rule yields

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}}[J(\Omega_{f,\boldsymbol{\theta}}, \boldsymbol{v}(\Omega_{f,\boldsymbol{\theta}}), p(\Omega_{f,\boldsymbol{\theta}}))] &= \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}}[\mathfrak{J}(\boldsymbol{\theta}, \boldsymbol{v}(\Omega_{f,\boldsymbol{\theta}}) \circ (I + \boldsymbol{\theta}), p(\Omega_{f,\boldsymbol{\theta}}) \circ (I + \boldsymbol{\theta}))] \\
&= \frac{\partial \mathfrak{J}}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}) + \frac{\partial \mathfrak{J}}{(\partial \hat{\boldsymbol{v}}, \hat{p})}(\dot{\boldsymbol{v}}, \dot{p}),
\end{aligned}
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$$= \frac{\partial \mathfrak{J}}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}) + \frac{\partial \mathfrak{J}}{(\partial \hat{\boldsymbol{v}}, \hat{p})}(\dot{\boldsymbol{v}}, \dot{p}),$$

where $(\dot{\boldsymbol{v}}, \dot{p}) = \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}}(\boldsymbol{v}(\Omega_{f,\boldsymbol{\theta}}) \circ (I+\boldsymbol{\theta}), p(\Omega_{f,\boldsymbol{\theta}}) \circ (I+\boldsymbol{\theta}))$ are the **Lagrangian derivatives** of $\boldsymbol{v}$ and p.

Shape derivatives for laminar flows

$(\boldsymbol{v}, p)$ are the solutions to find $(\boldsymbol{v}, p) \in \boldsymbol{v}_0 + V_{\boldsymbol{v},p}(\Gamma)$ such that

$$\forall (\boldsymbol{w}', q') \in V_{\boldsymbol{v},p}(\Gamma) \quad \int_{\Omega_f} \left[\nabla \boldsymbol{v} : \nabla \boldsymbol{w}' - p\mathrm{div}(\boldsymbol{w}') - q'\mathrm{div}(\boldsymbol{v})\right] \mathrm{d}x = \int_{\Omega_f} \boldsymbol{f}_f \cdot \boldsymbol{w}' \mathrm{d}x;$$

where $V_{\boldsymbol{v},p}(\Gamma) = \{(\boldsymbol{w}', q') \in H^1(\Omega_f, \mathbb{R}^d) \times L^2(\Omega_f)/\mathbb{R} \,|\, \boldsymbol{w} = 0 \text{ on } \partial\Omega_f\}$.

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$$\begin{aligned}\int_{\Omega_f} [\nabla \dot{\boldsymbol{v}} : \nabla \boldsymbol{w}' - \dot{p}\mathrm{div}(\boldsymbol{w}') - q'\mathrm{div}(\dot{v})]\mathrm{d}x = \int_{\Omega_f} [(\nabla \boldsymbol{v} \nabla \boldsymbol{\theta}) : \nabla \boldsymbol{w}' + \nabla \boldsymbol{v} : (\nabla \boldsymbol{w}' \nabla \boldsymbol{\theta}) \\ - p\mathrm{Tr}(\nabla \boldsymbol{w}' \nabla \boldsymbol{\theta}) - q'\mathrm{Tr}(\nabla \boldsymbol{v} \nabla \boldsymbol{\theta}) - (\nabla \boldsymbol{v} : \nabla \boldsymbol{w}' - p\mathrm{div}(\boldsymbol{w}') - \boldsymbol{f}_f \cdot \boldsymbol{w}')\mathrm{div}(\boldsymbol{\theta}) \\ + \boldsymbol{w}' \cdot (\nabla \boldsymbol{f}_f \, \boldsymbol{\theta})]\mathrm{d}x\end{aligned}$$

for all $(\boldsymbol{w}', q') \in V_{\boldsymbol{v},p}(\Gamma)$.

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for all $(\boldsymbol{w}', q') \in V_{\boldsymbol{v},p}(\Gamma)$. We introduce $(\boldsymbol{w}, q)$ the adjoint state solution to

$$\int_{\Omega_f} [\nabla \boldsymbol{w} : \nabla \boldsymbol{w}' - q\,\mathrm{div}(\boldsymbol{w}') - q'\mathrm{div}(\boldsymbol{w})]\mathrm{d}x = \frac{\partial \mathfrak{J}}{(\partial \hat{\boldsymbol{v}}, \partial \hat{p})}(w', q')$$

The chain rule yields

$$\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}}[J(\Omega_{f,\boldsymbol{\theta}}, \boldsymbol{v}(\Omega_{f,\boldsymbol{\theta}}), p(\Omega_{f,\boldsymbol{\theta}}))] = \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}}[\mathfrak{J}(\boldsymbol{\theta}, \boldsymbol{v}(\Omega_{f,\boldsymbol{\theta}}) \circ (\boldsymbol{I} + \boldsymbol{\theta}), p(\Omega_{f,\boldsymbol{\theta}}) \circ (\boldsymbol{I} + \boldsymbol{\theta}))]$$
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Proposition 5

Assume that the transported objective function $\mathfrak{J}(\boldsymbol{\theta}, \hat{\boldsymbol{v}}, \hat{p}) = J(\Omega_{f,\boldsymbol{\theta}}, \hat{\boldsymbol{v}} \circ (I+\boldsymbol{\theta})^{-1}, \hat{p} \circ (I+\boldsymbol{\theta})^{-1})$*, has continuous partial derivatives at* $(\boldsymbol{\theta}, \hat{\boldsymbol{v}}, \hat{p}) = (0, \boldsymbol{v}(\Omega_f), p(\Omega_f))$*. Then the objective function* $J(\Omega_f, \boldsymbol{v}(\Omega_f), p(\Omega_f))$ *is shape differentiable and the derivative reads*

$$
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& - p \mathrm{Tr}(\nabla \boldsymbol{w} \nabla \boldsymbol{\theta}) - q \mathrm{Tr}(\nabla \boldsymbol{v} \nabla \boldsymbol{\theta}) - (\nabla \boldsymbol{v} : \nabla \boldsymbol{w} - p \mathrm{div}(\boldsymbol{w}) - \boldsymbol{f}_f \cdot \boldsymbol{w}) \mathrm{div}(\boldsymbol{\theta}) \\
& + \boldsymbol{w} \cdot (\nabla \boldsymbol{f}_f \, \boldsymbol{\theta})] \mathrm{d}x.
\end{aligned}
$$

where $(\boldsymbol{w}, q)$ *is the adjoint state solution to*

$$
\int_{\Omega_f} [\nabla \boldsymbol{w} : \nabla \boldsymbol{w}' - q \mathrm{div}(\boldsymbol{w}') - q' \mathrm{div}(\boldsymbol{w})] \mathrm{d}x = \frac{\partial \mathfrak{J}}{(\partial \hat{\boldsymbol{v}}, \partial \hat{p})}(w', q')
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- These formulas require only the knowledge of $\partial \mathfrak{J}/\partial \boldsymbol{\theta}$ and $\partial \mathfrak{J}/\partial(\hat{\boldsymbol{v}}, \hat{p})$

Proposition 5

Assume that the transported objective function $\mathfrak{J}(\boldsymbol{\theta}, \hat{\boldsymbol{v}}, \hat{p}) = J(\Omega_{f,\boldsymbol{\theta}}, \hat{\boldsymbol{v}} \circ (I+\boldsymbol{\theta})^{-1}, \hat{p} \circ (I+\boldsymbol{\theta})^{-1})$*, has continuous partial derivatives at* $(\boldsymbol{\theta}, \hat{\boldsymbol{v}}, \hat{p}) = (0, \boldsymbol{v}(\Omega_f), p(\Omega_f))$*. Then the objective function* $J(\Omega_f, \boldsymbol{v}(\Omega_f), p(\Omega_f))$ *is shape differentiable and the derivative reads*

$$\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}}[J(\Omega_{f,\boldsymbol{\theta}}, \boldsymbol{v}(\Omega_{f,\boldsymbol{\theta}}), p(\Omega_{f,\boldsymbol{\theta}}))] = \frac{\partial \mathfrak{J}}{\partial \boldsymbol{\theta}} + \int_{\Omega_f} [(\nabla \boldsymbol{v} \nabla \boldsymbol{\theta}) : \nabla \boldsymbol{w} + \nabla \boldsymbol{v} : (\nabla \boldsymbol{w} \nabla \boldsymbol{\theta})$$
$$- p \mathrm{Tr}(\nabla \boldsymbol{w} \nabla \boldsymbol{\theta}) - q \mathrm{Tr}(\nabla \boldsymbol{v} \nabla \boldsymbol{\theta}) - (\nabla \boldsymbol{v} : \nabla \boldsymbol{w} - p \mathrm{div}(\boldsymbol{w}) - \boldsymbol{f}_f \cdot \boldsymbol{w}) \mathrm{div}(\boldsymbol{\theta})$$
$$+ \boldsymbol{w} \cdot (\nabla \boldsymbol{f}_f \, \boldsymbol{\theta})] \mathrm{d}x.$$

where $(\boldsymbol{w}, q)$ *is the adjoint state solution to*

$$\int_{\Omega_f} [\nabla \boldsymbol{w} : \nabla \boldsymbol{w}' - q \mathrm{div}(\boldsymbol{w}') - q' \mathrm{div}(\boldsymbol{w})] \mathrm{d}x = \frac{\partial \mathfrak{J}}{(\partial \hat{\boldsymbol{v}}, \partial \hat{p})}(w', q')$$

- These formulas require only the knowledge of $\partial \mathfrak{J} / \partial \boldsymbol{\theta}$ and $\partial \mathfrak{J} / \partial (\hat{\boldsymbol{v}}, \hat{p})$
- They can be implemented in a fully automated fashion.

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- They can be implemented in a fully automated fashion.
- This is a **volume form** of the shape derivative.

Example, the drag force:

$$\texttt{DRAG}(\Omega_f, \boldsymbol{v}(\Omega_f)) = \int_{\Omega_f} \nabla \boldsymbol{v} : \nabla \boldsymbol{v} \mathrm{d}x.$$

We find that

$$\frac{\partial \mathfrak{J}}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}) = \int_{\Omega_f} (-2(\nabla \boldsymbol{v} \nabla \boldsymbol{\theta}) : \nabla \boldsymbol{v} + \mathrm{div}(\boldsymbol{\theta}) \nabla \boldsymbol{v} : \nabla \boldsymbol{v}) \mathrm{d}x,$$

$$\frac{\partial \mathfrak{J}}{\partial (\hat{\boldsymbol{v}}, \hat{p})}(\boldsymbol{w}', q') = 2 \int_{\Omega_f} \nabla \boldsymbol{v} : \nabla \boldsymbol{w}' \mathrm{d}x.$$

It is also possible to write a generic formula in surface form.

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Proposition 6

Assume that the state and adjoint variables $(\boldsymbol{v}, p), (\boldsymbol{w}, q)$ *have* $H^2 \times H^1$ *regularity on* Ω_f *and that there exist* $\boldsymbol{f}_{\mathfrak{J}} \in L^1(D, \mathbb{R}^d)$ *and* $\boldsymbol{g}_{\mathfrak{J}} \in L^1(\Gamma, \mathbb{R}^d)$ *such that*

$$\forall \boldsymbol{\theta} \in W_0^{1,\infty}(D, \mathbb{R}^d), \; \frac{\partial \mathfrak{J}}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}) = \int_D \boldsymbol{f}_{\mathfrak{J}} \cdot \boldsymbol{\theta} \mathrm{d}x + \int_\Gamma \boldsymbol{g}_{\mathfrak{J}} \cdot \boldsymbol{\theta} \mathrm{d}\sigma.$$

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Then the shape derivative of $J(\Omega_f, \boldsymbol{v}(\Omega_f)$ *rewrites as an integral over the interface* Γ *depending only on* $\boldsymbol{\theta} \cdot \boldsymbol{n}$*:*

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}}\Big[J(\Omega_{f,\boldsymbol{\theta}}, \boldsymbol{v}(\Omega_{f,\boldsymbol{\theta}}), p(\Omega_{f,\boldsymbol{\theta}}), T(\Omega_{f,\boldsymbol{\theta}}), \boldsymbol{u}(\Omega_{f,\boldsymbol{\theta}}))\Big](\boldsymbol{\theta}) \\ &= \overline{\frac{\partial \mathfrak{J}}{\partial \boldsymbol{\theta}}}(\boldsymbol{\theta}) + \int_\Gamma (\boldsymbol{f}_f \cdot \boldsymbol{w} - \sigma_f(\boldsymbol{v}, p) : \nabla \boldsymbol{w} + \boldsymbol{n} \cdot \sigma_f(\boldsymbol{w}, q) \nabla \boldsymbol{v} \cdot \boldsymbol{n} + \boldsymbol{n} \cdot \sigma_f(\boldsymbol{v}, p) \nabla \boldsymbol{w} \cdot \boldsymbol{n})(\boldsymbol{\theta} \cdot \boldsymbol{n}) \mathrm{d}\sigma\end{aligned}$$

It is also possible to write a generic formula in surface form.

Proposition 6

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$$= \overline{\frac{\partial \mathfrak{J}}{\partial \boldsymbol{\theta}}}(\boldsymbol{\theta}) + \int_\Gamma (\boldsymbol{f}_f \cdot \boldsymbol{w} - \sigma_f(\boldsymbol{v}, p) : \nabla \boldsymbol{w} + \boldsymbol{n} \cdot \sigma_f(\boldsymbol{w}, q) \nabla \boldsymbol{v} \cdot \boldsymbol{n} + \boldsymbol{n} \cdot \sigma_f(\boldsymbol{v}, p) \nabla \boldsymbol{w} \cdot \boldsymbol{n})(\boldsymbol{\theta} \cdot \boldsymbol{n}) \mathrm{d}\sigma$$

where

$$\forall \boldsymbol{\theta} \in W_0^{1,\infty}(D, \mathbb{R}^d), \quad \overline{\frac{\partial \mathfrak{J}}{\partial \boldsymbol{\theta}}}(\boldsymbol{\theta}) := \int_\Gamma (\boldsymbol{g}_{\mathfrak{J}} \cdot \boldsymbol{n})(\boldsymbol{\theta} \cdot \boldsymbol{n}) \mathrm{d}\sigma,$$

is the part of $\frac{\partial \mathfrak{J}}{\partial \boldsymbol{\theta}}$ *that depends only on* $\boldsymbol{\theta} \cdot \boldsymbol{n}$*.*

Shape derivatives for laminar flows

Example, the drag force:

$$\mathtt{DRAG}(\Omega_f, \boldsymbol{v}(\Omega_f)) = \int_{\Omega_f} \nabla \boldsymbol{v} : \nabla \boldsymbol{v} \mathrm{d}x.$$

We find that

$$\frac{\partial \mathfrak{J}}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}) = \int_{\Omega_f} (-2(\nabla \boldsymbol{v} \nabla \boldsymbol{\theta}) : \nabla \boldsymbol{v} + \mathrm{div}(\boldsymbol{\theta}) \nabla \boldsymbol{v} : \nabla \boldsymbol{v}) \mathrm{d}x,$$

$$\frac{\partial \mathfrak{J}}{\partial (\hat{\boldsymbol{v}}, \hat{p})}(\boldsymbol{w}', q') = 2 \int_{\Omega_f} \nabla \boldsymbol{v} : \nabla \boldsymbol{w}' \mathrm{d}x.$$

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$$\overline{\frac{\partial \mathfrak{J}}{\partial \boldsymbol{\theta}}}(\boldsymbol{\theta}) = \int_{\partial \Omega_f} (-2(\nabla \boldsymbol{v}\, \boldsymbol{n})^2 + \nabla \boldsymbol{v} : \nabla \boldsymbol{v}) \boldsymbol{\theta} \cdot \boldsymbol{n} \mathrm{d}\sigma$$

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$$= -\int_{\partial \Omega_f} (\nabla \boldsymbol{v} : \nabla \boldsymbol{v}) \boldsymbol{\theta} \cdot \boldsymbol{n} \mathrm{d}\sigma.$$

Exercise:

- complete the derivation of shape derivative of arbitrary functionals for the linear elasticity system
- do the same for the heat conduction problem

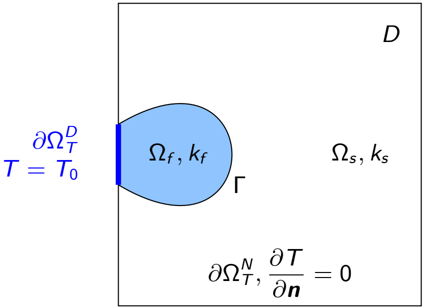

Figure: A bi-material distrubution of two conductive media with conductivity k_s and k_v.

$$\begin{cases} -\mathrm{div}(k_f \nabla T_f) = Q_f & \text{in } \Omega_f \\ -\mathrm{div}(k_s \nabla T_s) = Q_s & \text{in } \Omega_s \\ T = T_0 & \text{on } \partial\Omega_T^D \\ -k_f \dfrac{\partial T_f}{\partial \boldsymbol{n}} = h & \text{on } \partial\Omega_T^N \cap \partial\Omega_f \\ -k_s \dfrac{\partial T_s}{\partial \boldsymbol{n}} = h & \text{on } \partial\Omega_T^N \cap \partial\Omega_s \\ T_f = T_s & \text{on } \Gamma \\ -k_f \dfrac{\partial T_f}{\partial \boldsymbol{n}} = -k_s \dfrac{\partial T_s}{\partial \boldsymbol{n}} & \text{on } \Gamma, \end{cases}$$