Optimal Shape Design of Air Ducts in Combustion Engines

Design a General Shape Optimization Framework

Michael Hintermüller   Hồng Quản Bá Nguyễn

Weierstrass Institute for Applied Analysis & Stochastics (WIAS Berlin)

Joint work with Karl Knall

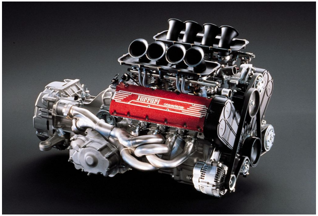
Reduced Order Modelling, Simulation and Optimization of Coupled Systems (ROMSOC)

Berlin, 5th August 2021

Funded by the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie Grant Agreement No. 765374.

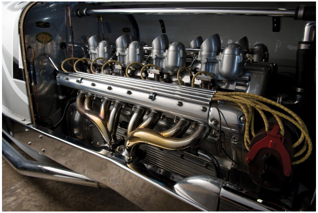
Combustion engines

(a) Toyota car.



(b) Ferrari combustion engine.

(c) BMW combustion engine.



(d) A beautiful combustion engine.

- A schematic 1-inlet-1-outlet duct geometry & its boundary:

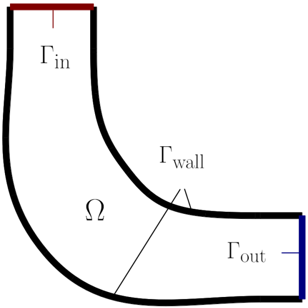


Figure: A simple sketch of a 1-inlet-1-outlet air duct.

- Air ducts with multiple inlets &/or outlets $\to$ later.
- **Target.** $\boxed{\text{Optimize the shape of air ducts.}}$

A BVP for the instationary incompressible viscous NSEs with *mixed boundary conditions*:

$$\begin{cases} \mathbf{u}_t - \nu\Delta\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = \mathbf{f} & \text{in } (0,T)\times\Omega, \\ \nabla\cdot\mathbf{u} = 0 & \text{in } (0,T)\times\Omega, \\ \mathbf{u}(0,\cdot) = \mathbf{u}_0 & \text{in } \Omega, \\ \mathbf{u} = \mathbf{f}_{\mathrm{in}} & \text{on } [0,T]\times\Gamma_{\mathrm{in}}, \\ \mathbf{u} = \mathbf{0} & \text{on } [0,T]\times\Gamma_{\mathrm{wall}}, \\ -\nu\partial_{\mathbf{n}}\mathbf{u} + p\mathbf{n} = \mathbf{0} & \text{on } [0,T]\times\Gamma_{\mathrm{out}}, \end{cases} \tag{iNS}$$

where

- $\mathbf{u} : [0,T]\times\Omega \to \mathbb{R}^N$: velocity, $p : [0,T]\times\Omega \to \mathbb{R}$: pressure;
- $\nu > 0$: kinematic viscosity, $\mathbf{f}$: source term, $\mathbf{u}_0$: initial velocity, $\mathbf{f}_{\mathrm{in}}$: inflow profile at Γ_{in}.

- **Flow uniformity at the outlet.**
  - An important design criterion of *automotive air ducts*.
  - Efficiently distribute fresh air inside cars/engines.

$$J_1(\mathbf{u}, \Omega) := \frac{1}{2} \int_0^T \int_{\Gamma_{\mathrm{out}}} (\mathbf{u} \cdot \mathbf{n} - \overline{u})^2 \, \mathrm{d}\Gamma \mathrm{d}t, \tag{J_1}$$

with a desired value $\overline{u}$, e.g.:

$$\overline{u} := -\frac{1}{T H_{N-1}(\Gamma_{\mathrm{out}})} \int_0^T \int_{\Gamma_{\mathrm{in}}} \mathbf{f}_{\mathrm{in}} \cdot \mathbf{n} \mathrm{d}\Gamma \mathrm{d}t,$$

where $H_{N-1}(\cdot)$: $(N-1)$-dimensional Hausdorff measure.

- **Energy dissipation.**
  - Minimize the power dissipated by air ducts/any fluid dynamics devices.
  - Compute the dissipated power as the net inward flux of energy through the boundary:

$$J_2(\mathbf{u}, p, \Omega) := -\int_0^T \int_\Gamma \left(p + \frac{1}{2}|\mathbf{u}|^2\right) \mathbf{u} \cdot \mathbf{n} \,\mathrm{d}\Gamma \mathrm{d}t. \tag{J_2}$$

Regularity of (iNS). $(\mathbf{u}, p) \in W^{1,2}(\Omega; \mathbb{R}^N) \times L^2(\Omega)$ usually [MR2009].
Consider an approximation of J_2, with thickness $\delta > 0$:

$$\begin{aligned} J_2^\delta(\mathbf{u}, p, \Omega) := &-\frac{H_{N-1}(\Gamma_{\mathrm{in}})}{\mathrm{m}_N(\Gamma_{\mathrm{in}}^\delta)} \int_0^T \int_{\Gamma_{\mathrm{in}}^\delta} \left(p + \frac{1}{2}|\mathbf{u}|^2\right) \mathbf{u} \cdot \mathbf{n} \,\mathrm{d}\mathbf{x} \mathrm{d}t \\ &- \frac{H_{N-1}(\Gamma_{\mathrm{out}})}{\mathrm{m}_N(\Gamma_{\mathrm{out}}^\delta)} \int_0^T \int_{\Gamma_{\mathrm{out}}^\delta} \left(p + \frac{1}{2}|\mathbf{u}|^2\right) \mathbf{u} \cdot \mathbf{n} \,\mathrm{d}\mathbf{x} \mathrm{d}t. \end{aligned} \tag{J_2^δ}$$

$$J_2^\delta(\mathbf{u}, p, \Omega) = \int_0^T \int_\Omega k_\delta(\mathbf{x}) \left(p + \frac{1}{2}|\mathbf{u}|^2 \right) \mathbf{u} \cdot \mathbf{n} \mathrm{d}\mathbf{x} \mathrm{d}t,$$

where m_N denotes the N-dimensional Lebesgue measure &

$$k_\delta(\mathbf{x}) := -\frac{H_{N-1}(\Gamma_{\mathrm{in}})}{\mathrm{m}_N(\Gamma_{\mathrm{in}}^\delta)} \chi_{\Gamma_{\mathrm{in}}^\delta}(\mathbf{x}) - \frac{H_{N-1}(\Gamma_{\mathrm{out}})}{\mathrm{m}_N(\Gamma_{\mathrm{out}}^\delta)} \chi_{\Gamma_{\mathrm{out}}^\delta}(\mathbf{x}), \ \forall \mathbf{x} \in \Omega.$$

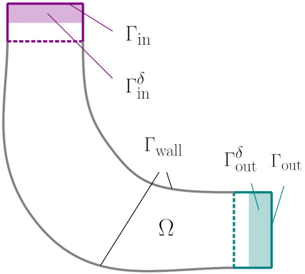


Figure: The duct geometry with δ-approximated inlet $\Gamma_{\mathrm{in}}^\delta$ & outlet $\Gamma_{\mathrm{out}}^\delta$.

Mixed cost functional & a shape optimization problem

A mixed cost functional with a weighting parameter $\gamma \in [0,1]$:

$$
\begin{aligned}
J_{12}^{\delta,\gamma}(\mathbf{u},p,\Omega) &\coloneqq (1-\gamma)J_1(\mathbf{u},\Omega) + \gamma J_2^{\delta}(\mathbf{u},p,\Omega) \\
&= \frac{1-\gamma}{2}\int_0^T \int_{\Gamma_{\mathrm{out}}} (\mathbf{u}\cdot\mathbf{n} - \overline{u})^2 \,\mathrm{d}\Gamma\mathrm{d}t \\
&\quad + \int_0^T \int_{\Omega} \gamma k_\delta(\mathbf{x}) \left(p + \frac{1}{2}|\mathbf{u}|^2\right) \mathbf{u}\cdot\mathbf{n}\mathrm{d}\mathbf{x}\mathrm{d}t.
\end{aligned}
\tag{$J_{12}^{\delta,\gamma}$}
$$

A PDEs-constrained shape optimization problem (SOP):

$$
\boxed{\min_{\Omega\in\mathcal{O}_{\mathrm{ad}}} J_{12}^{\delta,\gamma}(\mathbf{u},p,\Omega) \text{ s.t. } (\mathbf{u},p) \text{ solves (iNS).}} \tag{sop}
$$

Targets

- Topology Optimization [later] & Shape Optimization for BVPs of
  - Stationary Navier-Stokes equations
  - Instationary Navier-Stokes equations
  - Large Eddy Simulation (LES), e.g., Smagorinsky turbulence model
  - Reynolds-averaged Navier-Stokes (RANS) equations, e.g., k-ϵ turbulence model [MP1994]

  in 2D & 3D with mixed boundary conditions.
- Develop FEM/FVM-based (e.g., FEniCS/OpenFOAM-based) software to implement the continuous adjoint approach.

A general model & cost/shape functional

- A general stationary PDEs for velocity $\mathbf{u}$ & pressure p:

$$\boxed{\begin{cases} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p) = \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) & \text{in } \Omega, \\ -\nabla\cdot\mathbf{u} = f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) & \text{in } \Omega, \\ \mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) = \mathbf{f}_{\mathrm{bc}}(\mathbf{x}) & \text{on } \Gamma, \end{cases}} \tag{gfld}$$

  where $\mathbf{P}(\cdot, \ldots, \cdot)$ denotes the main PDEs (e.g., momentum conservation equations), $\mathbf{Q}(\cdot, \ldots, \cdot)$ denotes the boundary conditions (BCs).
- A general cost functional for (gfld):

$$\boxed{J(\mathbf{u}, p, \Omega) := \int_\Omega J_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\mathrm{d}\mathbf{x} + \int_\Gamma J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})\mathrm{d}\Gamma.} \tag{cost-gfld}$$

Lagrangians

To derive the adjoint equations for (gfld), introduce:

- **Standard Lagrangian**:

$$\begin{aligned} &L(\mathbf{u}, p, \Omega, \mathbf{v}, q) \\ &:= J(\mathbf{u}, p, \Omega) + \int_\Omega -\left(\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p) - \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\right) \cdot \mathbf{v} \\ &\qquad + q\left(\nabla \cdot \mathbf{u} + f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\right) \mathrm{d}\mathbf{x}. \end{aligned} \tag{L-gfld}$$

- **Extended Lagrangian**:

$$\begin{aligned} &\mathcal{L}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\mathrm{bc}}) \\ &:= L(\mathbf{u}, p, \Omega, \mathbf{v}, q) - \int_\Gamma \left(\mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) - \mathbf{f}_{\mathrm{bc}}(\mathbf{x})\right) \cdot \mathbf{v}_{\mathrm{bc}} \mathrm{d}\Gamma. \end{aligned} \tag{$\mathcal{L}$-gfld}$$

where $\mathbf{v}$, q, $\mathbf{v}_{\mathrm{bc}}$ are Lagrange multipliers.

Consider 3 different SOPs for (cost-gfld), (L-gfld), & ($\mathcal{L}$-gfld), resp.:

- Treat the whole of (gfld) as equality constraints:

$$\boxed{\min_{\Omega\in\mathcal{O}_{\mathrm{ad}}} J(\mathbf{u}, p, \Omega) \text{ s.t. } (\mathbf{u}, p) \text{ solves (gfld)},} \tag{sop-J-gfld}$$

- Penalize the 1st 2 equations of (gfld) but keep the BCs as an equality constraint:

$$\boxed{\min_{\Omega\in\mathcal{O}_{\mathrm{ad}}} L(\mathbf{u}, p, \Omega, \mathbf{v}, q) \text{ s.t. } (\mathbf{u}, p) \text{ s.t. } \mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) = \mathbf{f}_{\mathrm{bc}}(\mathbf{x}) \text{ on } \Gamma,} \tag{sop-L-gfld}$$

- Penalize all of (gfld):

$$\boxed{\min_{\Omega\in\mathcal{O}_{\mathrm{ad}}} \mathcal{L}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\mathrm{bc}}) \text{ with } (\mathbf{u}, p) \text{ unconstrained.}} \tag{sop-$\mathcal{L}$-gfld}$$

- **Question.** *Use standard/extended Lagrangian to derive adjoint PDEs?*
- Consider a "mixed Lagrangian" with a "switch" $\delta_{\mathcal{L}} \in \{0, 1\}$:

$$L_{\mathcal{L}}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc}) := L - \delta_{\mathcal{L}} \int_{\Gamma} (\mathbf{Q} - \mathbf{f}_{\rm bc}) \cdot \mathbf{v}_{\rm bc} \mathrm{d}\Gamma. \qquad (\mathcal{L}\text{-gfld})$$

Hence,

$$L_{\mathcal{L}}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc}) = \begin{cases} L(\mathbf{u}, p, \Omega, \mathbf{v}, q) & \text{if } \delta_{\mathcal{L}} = 0, \\ \mathcal{L}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc}) & \text{if } \delta_{\mathcal{L}} = 1. \end{cases}$$

- 4th SOP (a combination of 2nd & 3rd SOPs):

$$\boxed{\min_{\Omega \in \mathcal{O}_{\rm ad}} L_{\mathcal{L}}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc}) \begin{cases} \text{s.t. } (\mathbf{u}, p) \text{ s.t. } \mathbf{Q} = \mathbf{f}_{\rm bc} \text{ on } \Gamma & \text{if } \delta_{\mathcal{L}} = 0, \\ \text{with } (\mathbf{u}, p) \text{ unconstrained} & \text{if } \delta_{\mathcal{L}} = 1. \end{cases}}$$

(sop-$L_{\mathcal{L}}$-gfld)

Derive adjoint PDEs

- Formally, if $(\mathbf{u}^\star, p^\star, \Omega^\star)$ is an optimal point, then

$$D_{(\mathbf{u},p)} L_{\mathcal{L}}(\mathbf{u}^\star, p^\star, \Omega^\star, \mathbf{v}, q, \mathbf{v}_{\mathrm{bc}})(\tilde{\mathbf{u}}, \tilde{p}) = 0, \ \forall (\tilde{\mathbf{u}}, \tilde{p}).$$

- Choose the adjoint variables/Lagrange multipliers $(\mathbf{v}, q, \mathbf{v}_{\mathrm{bc}})$ s.t.

$$\boxed{D_{\mathbf{u}} L_{\mathcal{L}}(\mathbf{u}^\star, p^\star, \Omega^\star, \mathbf{v}, q, \mathbf{v}_{\mathrm{bc}})\tilde{\mathbf{u}} + D_p L_{\mathcal{L}}(\mathbf{u}^\star, p^\star, \Omega^\star, \mathbf{v}, q, \mathbf{v}_{\mathrm{bc}})\tilde{p} = 0,}$$

for all $(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}, \tilde{p})$, where $\tilde{\mathbf{u}}$, $\tilde{p}$: variations of $\mathbf{u}$, p, resp.

- Expand this explicitly, $\forall (\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}, \tilde{p})$:

$$\int_\Omega \left[F_\Omega^{\Delta\tilde{\mathbf{u}}}(\cdot)\Delta\tilde{\mathbf{u}} + F_\Omega^{\nabla\tilde{\mathbf{u}}}(\cdot)\nabla\tilde{\mathbf{u}} + F_\Omega^{\tilde{\mathbf{u}}}(\cdot)\tilde{\mathbf{u}} + F_\Omega^{\tilde{p}}(\cdot)\tilde{p} + F_\Omega^{\nabla\tilde{p}}(\cdot)\nabla\tilde{p} \right] \cdot \{\mathbf{v}, q\} \mathrm{d}\mathbf{x}$$

$$+ D_{(\mathbf{u},p)} J(\mathbf{u}, p, \Omega)(\tilde{\mathbf{u}}, \tilde{p}) + \delta_{\mathcal{L}} \int_\Gamma \left[F_\Gamma^{\nabla\tilde{\mathbf{u}}}(\cdot)\nabla\tilde{\mathbf{u}} + F_\Gamma^{\tilde{\mathbf{u}}}(\cdot)\tilde{\mathbf{u}} + F_\Gamma^{\tilde{p}}(\cdot)\tilde{p} \right] \cdot \mathbf{v}_{\mathrm{bc}} \mathrm{d}\Gamma$$

$$= 0, \ \text{where } (\cdot)|_\Omega = (\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p), \ (\cdot)|_\Gamma = (\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}, \mathbf{v}_{\mathrm{bc}}).$$

Derive adjoint of (gfld): integrate by parts

- Let $A : D(A) \subset E \to F$: an unbounded linear operator [Brezis2010]. Adjoint of A: the unbounded linear operator $A^\star : D(A^\star) \subset F^\star \to E^\star$ s.t.

$$\langle v, Au \rangle_{F^\star, F} = \langle A^\star v, u \rangle_{E^\star, E}, \ \forall u \in D(A), \ \forall v \in D(A^\star).$$

- Analogously, rewrite the current equation:

$$\begin{aligned}&(1, A_{J_\Omega}(\tilde{\mathbf{u}}, \tilde{p}))_{L^2(\Omega)} + (1, A_{J_\Gamma}(\tilde{\mathbf{u}}, \tilde{p}))_{L^2(\Gamma)} + ((\mathbf{v}, q), A_\Omega(\tilde{\mathbf{u}}, \tilde{p}))_{L^2(\Omega)} \\ &\quad + \delta_{\mathcal{L}} (\mathbf{v}_{\mathrm{bc}}, A_\Gamma(\tilde{\mathbf{u}}, \tilde{p}))_{L^2(\Gamma)} = 0, \ \forall (\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}, \tilde{p}).\end{aligned}$$

- **Goal.** Integrate by parts to obtain:

$$\begin{aligned}&\left(A^\star_{J_\Omega} 1, (\tilde{\mathbf{u}}, \tilde{p})\right)_{L^2(\Omega)} + (1, A_{J_\Gamma}(\tilde{\mathbf{u}}, \tilde{p}))_{L^2(\Gamma)} + (A^\star_\Omega(\mathbf{v}, q), (\tilde{\mathbf{u}}, \tilde{p}))_{L^2(\Omega)} \\ &\quad + \delta_{\mathcal{L}} (\mathbf{v}_{\mathrm{bc}}, A_\Gamma(\tilde{\mathbf{u}}, \tilde{p}))_{L^2(\Gamma)} = 0, \ \forall (\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}, \tilde{p}).\end{aligned}$$

- **Question.** *Integrate by parts which terms?*

Derive adjoint of (gfld): integrate by parts

- Roughly speaking,

$$\int_\Omega F_\Omega\{\nabla\tilde{\mathbf{u}}, \Delta\tilde{\mathbf{u}}, \nabla\tilde{p}\}\cdot\{\mathbf{v}, q\}\mathrm{d}\mathbf{x} \xrightarrow{\text{i.b.p.}} \int_\Omega \{\tilde{\mathbf{u}}, \tilde{p}\}\cdot F_\Omega^\star\{\nabla\mathbf{v}, \Delta\mathbf{v}, \nabla q\}\mathrm{d}\mathbf{x} + \text{ by-products } \int_\Gamma \cdots \mathrm{d}\Gamma.$$

- Integrate by parts all the red terms:

$$\begin{aligned}&\int_\Omega \left[F_\Omega^{\Delta\tilde{\mathbf{u}}}(\cdot)\Delta\tilde{\mathbf{u}} + F_\Omega^{\nabla\tilde{\mathbf{u}}}(\cdot)\nabla\tilde{\mathbf{u}} + F_\Omega^{\tilde{\mathbf{u}}}(\cdot)\tilde{\mathbf{u}} + F_\Omega^{\tilde{p}}(\cdot)\tilde{p} + F_\Omega^{\nabla\tilde{p}}(\cdot)\nabla\tilde{p}\right]\cdot\{\mathbf{v}, q\}\mathrm{d}\mathbf{x}\\ &+ \int_\Omega D_{\nabla\mathbf{u}}J_\Omega(\cdot)\nabla\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} + \text{ the rest of } D_{(\mathbf{u},p)}J(\mathbf{u}, p, \Omega)\\ &+ \delta_{\mathcal{L}}\int_\Gamma \left[F_\Gamma^{\nabla\tilde{\mathbf{u}}}(\cdot)\nabla\tilde{\mathbf{u}} + F_\Gamma^{\tilde{\mathbf{u}}}(\cdot)\tilde{\mathbf{u}} + F_\Gamma^{\tilde{p}}(\cdot)\tilde{p}\right]\cdot\mathbf{v}_{\mathrm{bc}}\mathrm{d}\Gamma = 0.\end{aligned}$$

Derive adjoint of (gfld) with extended Lagrangian ($\mathcal{L}$-gfld)

Assume $\delta_{\mathcal{L}} = 1$. Gather terms: $\forall(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}, \tilde{p})$,

$$\int_\Omega \mathbf{F}_\Omega^{\tilde{\mathbf{u}}}(\cdot) \cdot \tilde{\mathbf{u}} + F_\Omega^{\tilde{p}}(\cdot)\tilde{p}\mathrm{d}\mathbf{x} + \int_\Gamma \mathbf{F}_\Gamma^{\tilde{\mathbf{u}}}(\cdot) \cdot \tilde{\mathbf{u}} + F_\Gamma^{\tilde{p}}(\cdot)\tilde{p} + F_\Gamma^{\nabla\tilde{\mathbf{u}}}(\cdot, \nabla\tilde{\mathbf{u}})\mathrm{d}\Gamma = 0,$$

- Choose $\tilde{\mathbf{u}}|_{\overline{\Omega}} = \mathbf{0}$, $\int_\Omega F_\Omega^{\tilde{p}}(\cdot)\tilde{p}\mathrm{d}\mathbf{x} + \int_\Gamma F_\Gamma^{\tilde{p}}(\cdot)\tilde{p}\mathrm{d}\Gamma = 0$, $\forall(\mathbf{u}, p, \Omega, \tilde{p})$.
  - Choose $\tilde{p}$ s.t. $\tilde{p}|_\Gamma = 0$, then $\int_\Omega F_\Omega^{\tilde{p}}(\cdot)\tilde{p}\mathrm{d}\mathbf{x} = 0$ $\forall(\mathbf{u}, p, \Omega, \tilde{p})$ s.t. $\tilde{p}|_\Gamma = 0$, thus

$$\boxed{F_\Omega^{\tilde{p}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p, \mathbf{v}, \nabla\mathbf{v}, q) = 0 \text{ in } \Omega.}$$

  - Plug it back in, obtain $\int_\Gamma F_\Gamma^{\tilde{p}}(\cdot)\tilde{p}\mathrm{d}\Gamma = 0$, $\forall(\mathbf{u}, p, \Omega, \tilde{p})$, thus

$$\boxed{F_\Gamma^{\tilde{p}}(\cdot)(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p, \mathbf{v}, \mathbf{v}_{\mathrm{bc}}, \mathbf{n}, \mathbf{t}) = 0 \text{ on } \Gamma.}$$

Derive adjoint of (gfld) with extended Lagrangian ($\mathcal{L}$-gfld)

- Assume $(\mathbf{v}, q)$ satisfies these 2, then

$$\int_\Omega \mathbf{F}_\Omega^{\tilde{\mathbf{u}}}(\cdot) \cdot \tilde{\mathbf{u}} \mathrm{d}\mathbf{x} + \int_\Gamma \mathbf{F}_\Gamma^{\tilde{\mathbf{u}}}(\cdot) \cdot \tilde{\mathbf{u}} + F_\Gamma^{\nabla\tilde{\mathbf{u}}}(\cdot, \nabla\tilde{\mathbf{u}})\mathrm{d}\Gamma = 0, \ \forall(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}).$$

- Choose $\tilde{\mathbf{u}}$ s.t. $\tilde{\mathbf{u}}|_\Gamma = \mathbf{0}$ & $\nabla\tilde{\mathbf{u}}|_\Gamma = \mathbf{0}_{N\times N}$, then $\int_\Omega \mathbf{F}_\Omega^{\tilde{\mathbf{u}}}(\cdot) \cdot \tilde{\mathbf{u}} \mathrm{d}\mathbf{x} = 0$, thus

$$\boxed{\mathbf{F}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p, \mathbf{v}, \nabla\mathbf{v}, q, \nabla q) = \mathbf{0} \text{ in } \Omega.}$$

- Plug it back in, obtain $\int_\Gamma \mathbf{F}_\Gamma^{\tilde{\mathbf{u}}}(\cdot) \cdot \tilde{\mathbf{u}} \mathrm{d}\Gamma + \int_\Gamma F_\Gamma^{\nabla\tilde{\mathbf{u}}}(\cdot, \nabla\tilde{\mathbf{u}})\mathrm{d}\Gamma = 0$, $\forall(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}})$.
  - Choose $\tilde{\mathbf{u}}$ s.t. $\tilde{\mathbf{u}}|_\Gamma = \mathbf{0}$, $\int_\Gamma F_\Gamma^{\nabla\tilde{\mathbf{u}}}(\cdot, \nabla\tilde{\mathbf{u}})\mathrm{d}\Gamma = 0$, thus

$$\boxed{\begin{aligned}&\sum_{k=1}^N v_k \partial_{\Delta u_j} P_k(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p) n_i - \partial_{\partial_{x_i} u_j} Q_k(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) v_{\mathrm{bc},k} \\ &= -\partial_{\partial_{x_i} u_j} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}), \ \forall i, j = 1, \ldots, N.\end{aligned}}$$

  - Plug it back in, $\int_\Gamma \mathbf{F}_\Gamma^{\tilde{\mathbf{u}}}(\cdot) \cdot \tilde{\mathbf{u}} \mathrm{d}\Gamma = 0$, $\forall(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}})$, thus

$$\boxed{\mathbf{F}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p, \mathbf{v}, \nabla\mathbf{v}, q, \mathbf{v}_{\mathrm{bc}}, \mathbf{n}, \mathbf{t}) = \mathbf{0} \text{ on } \Gamma.}$$

Adjoint of (gfld)

$$
\begin{cases}
-\nabla_{\Delta \mathbf{u}} \mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta\mathbf{v} + (\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) - \nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)) : \nabla\mathbf{v} \\
\quad - [\nabla_{\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) + \Delta\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) - \nabla_{\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)]\,\mathbf{v} \\
\quad + [\nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)) - \nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))]\cdot\mathbf{v} - \nabla q \\
\quad - \nabla_{\nabla\mathbf{u}} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\nabla q + q\,[-\nabla\cdot(\nabla_{\nabla\mathbf{u}} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)) + \nabla_{\mathbf{u}} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)] \\
\qquad = \nabla\cdot(\nabla_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)) - \nabla_{\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) \text{ in } \Omega, \\
\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) : \nabla\mathbf{v} \\
\quad + [-D_p\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) + \nabla\cdot(\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)) + D_p\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)]\cdot\mathbf{v} \\
\qquad = -D_p J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) - qD_p f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) \text{ in } \Omega, \\
-\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\mathbf{v} + [(-\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) + \nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\cdot\mathbf{n}]\cdot\mathbf{v} \\
\quad - \partial_{\mathbf{n}}\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v} + q\mathbf{n} - \nabla_{\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{v}_{\mathrm{bc}} \\
\qquad = -\nabla_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n} - \nabla_{\mathbf{u}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) - q\nabla_{\nabla\mathbf{u}} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n} \text{ on } \Gamma, \\
\mathbf{n}^\top\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v} + D_p\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\mathbf{v}_{\mathrm{bc}} = D_p J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) \text{ on } \Gamma, \\
\displaystyle\sum_{k=1}^{N} v_k \partial_{\Delta u_j} P_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) n_i - \partial_{\partial_{x_i} u_j} Q_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) v_{\mathrm{bc},k} \\
\qquad = -\partial_{\partial_{x_i} u_j} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}),\ \forall i,j = 1,\ldots,N.
\end{cases}
$$

(ex-adj-gfld)

- Given $\emptyset \neq D \subset \mathbb{R}^N$ (underlying *holdall/universe*), consider a velocity field $V : [0,\tau] \times \overline{D} \to \mathbb{R}^N$ verifying Lipschitz & linear tangent space conditions (see [DZ2011]).
- Perturbed domain of a set $\Omega \subset \overline{D}$:

$$\Omega_t(V) \coloneqq T_t(V)(\Omega) = \{T_t(V)(X); \forall X \in \Omega\} \subset \overline{D},$$

where the transformation $T_t : \overline{D} \to \overline{D}$ is given by

$$T_t(X) \coloneqq x(t,X),\ t \geq 0,\ X \in \overline{D},\ \begin{cases} \dfrac{dx}{dt}(t,X) = V(t,x(t,X)),\ t \geq 0, \\ x(0,X) = X. \end{cases}$$

- Eulerian semiderivative of a shape functional $J : \mathcal{O}_{\mathrm{ad}} \subset 2^D \to \mathbb{R}$:

$$dJ(\Omega; V) = \lim_{t \downarrow 0} \frac{J(\Omega_t(V)) - J(\Omega)}{t}.$$

Theorem (Domain integrals [DZ2011])

Assume $\exists \tau > 0$ *s.t.* $V(t)$ *satisfies* (V), $V \in C^0([0,\tau]; C^1_{\mathrm{loc}}(\mathbb{R}^N, \mathbb{R}^N))$. *Given* $\varphi \in C(0,\tau; W^{1,1}_{\mathrm{loc}}(\mathbb{R}^N)) \cap C^1(0,\tau; L^1_{\mathrm{loc}}(\mathbb{R}^N))$, Ω*: a bounded measurable domain, the semiderivative of*

$$J_V(t) := \int_{\Omega_t(V)} \varphi(t)\mathrm{dx}$$

at $t = 0$ *is given by, with* $\varphi(0)(\mathrm{x}) := \varphi(0,\mathrm{x})$ *&* $\varphi'(0)(\mathrm{x}) := \partial_t\varphi(0,\mathrm{x})$*:*

$$dJ_V(0) = \int_\Omega \varphi'(0) + \nabla \cdot (\varphi(0)V(0))\,\mathrm{dx}.$$

If, in addition, Ω *is an open domain with a Lipschitzian boundary* Γ*, then*

$$dJ_V(0) = \int_\Omega \varphi'(0)\mathrm{dx} + \int_\Gamma \varphi(0)V(0)\cdot \mathrm{n}\mathrm{d}\Gamma.$$

Theorem (Boundary integrals [DZ2011])

Let $\Gamma := \partial\Omega$, $\Omega \subset \mathbb{R}^N$*: bounded open of class* C^2, $\psi \in C^1([0,\tau]; H^2_{\mathrm{loc}}(\mathbb{R}^N))$. *Assume* $V \in C^0([0,\tau]; C^1_{\mathrm{loc}}(\mathbb{R}^N,\mathbb{R}^N))$. *Consider the function*

$$J_V(t) := \int_{\Gamma_t(V)} \psi(t)\mathrm{d}\Gamma_t.$$

Then the derivative of $J_V(t)$ *w.r.t.* t *at* $t = 0$ *is given by:*

$$\begin{aligned} dJ_V(0) &= \int_\Gamma \psi'(0) + (\partial_{\mathrm{n}}\psi + H\psi)V(0)\cdot \mathrm{n}\mathrm{d}\Gamma \\ &= \int_\Gamma \psi'(0) + \nabla\psi \cdot V(0) + \psi\left(\nabla \cdot V(0) - DV(0)\mathrm{n}\cdot\mathrm{n}\right)\mathrm{d}\Gamma. \end{aligned}$$

where $\psi'(0)(\mathrm{x}) := \partial_t\psi(0,\mathrm{x})$.

1st-order shape derivatives of (gfld)-constrained (cost-gfld)

Recall (cost-gfld) & consider its perturbed analogue:

$$J(\mathbf{u}, p, \Omega) = \int_{\Omega} J_{\Omega}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p)\mathrm{d}\mathbf{x} + \int_{\Gamma} J_{\Gamma}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t})\mathrm{d}\Gamma,$$

$$J(\mathbf{u}_t, p_t, \Omega_t) = \int_{\Omega_t} J_{\Omega}(\mathbf{x}, \mathbf{u}_t, \nabla \mathbf{u}_t, p_t)\mathrm{d}\mathbf{x} + \int_{\Gamma_t} J_{\Gamma}(\mathbf{x}, \mathbf{u}_t, \nabla \mathbf{u}_t, p_t, \mathbf{n}_t, \mathbf{t}_t)\mathrm{d}\Gamma.$$

where $(\mathbf{u}_t, p_t)$ solves (gfld) on the perturbed domain $\Omega_t \coloneqq T_t(V)(\Omega)$:

$$\begin{cases} \mathbf{P}(\mathbf{x}, \mathbf{u}_t, \nabla \mathbf{u}_t, \Delta \mathbf{u}_t, p_t, \nabla p_t) = \mathbf{f}(\mathbf{x}, \mathbf{u}_t, \nabla \mathbf{u}_t, p_t) & \text{in } \Omega_t, \\ -\nabla \cdot \mathbf{u}_t = f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}_t, \nabla \mathbf{u}_t, p_t) & \text{in } \Omega_t, \\ \mathbf{Q}(\mathbf{x}, \mathbf{u}_t, \nabla \mathbf{u}_t, \Delta \mathbf{u}_t, p_t, \mathbf{n}_t, \mathbf{t}_t) = \mathbf{f}_{\mathrm{bc}}(\mathbf{x}) & \text{on } \Gamma_t. \end{cases} \qquad \text{(ptb-gfld)}$$

Define *local shape derivatives*:

$$\mathbf{u}'(\mathbf{x}; V) \coloneqq \lim_{t \downarrow 0} \frac{\mathbf{u}_t(\mathbf{x}) - \mathbf{u}(\mathbf{x})}{t}, \ \ p'(\mathbf{x}; V) \coloneqq \lim_{t \downarrow 0} \frac{p_t(\mathbf{x}) - p(\mathbf{x})}{t}, \ \ \forall \mathbf{x} \in D.$$

1st-order shape derivatives of (gfld)-constrained (cost-gfld)

- Subtract (ptb-gfld) to (gfld), take $\lim_{t\downarrow 0}$ to obtain

$$\boxed{\begin{cases} D_{\mathbf{u}}\mathbf{P}(\cdot)\mathbf{u}'(\mathbf{x};V) + D_{\nabla\mathbf{u}}\mathbf{P}(\cdot)\nabla\mathbf{u}'(\mathbf{x};V) + D_{\Delta\mathbf{u}}\mathbf{P}(\cdot)\Delta\mathbf{u}'(\mathbf{x};V) \\ \quad + D_p\mathbf{P}(\cdot)p'(\mathbf{x};V) + D_{\nabla p}\mathbf{P}(\cdot)\nabla p'(\mathbf{x};V) \\ \qquad = D_{\mathbf{u}}\mathbf{f}(\cdot)\mathbf{u}'(\mathbf{x};V) + D_{\nabla\mathbf{u}}\mathbf{f}(\cdot)\nabla\mathbf{u}'(\mathbf{x};V) + D_p\mathbf{f}(\cdot)p'(\mathbf{x};V) \text{ in } \Omega, \\ -\nabla\cdot\mathbf{u}'(\mathbf{x};V) = D_{\mathbf{u}}f_{\rm div}(\cdot)\mathbf{u}'(\mathbf{x};V) + D_{\nabla\mathbf{u}}f_{\rm div}(\cdot)\nabla\mathbf{u}'(\mathbf{x};V) \\ \qquad\qquad + D_p f_{\rm div}(\cdot)p'(\mathbf{x};V) \text{ in } \Omega, \\ D_{\mathbf{u}}\mathbf{Q}(\cdot)\mathbf{u}'(\mathbf{x};V) + D_{\nabla\mathbf{u}}\mathbf{Q}(\cdot)\nabla\mathbf{u}'(\mathbf{x};V) + D_p\mathbf{Q}(\cdot)p'(\mathbf{x};V) \\ \quad + D_{\mathbf{n}}\mathbf{Q}(\cdot)\mathbf{n}'(\mathbf{x};V) + D_{\mathbf{t}}\mathbf{Q}(\cdot)\mathbf{t}'(\mathbf{x};V) = 0 \text{ on } \Gamma. \end{cases}}$$

- Test this with the adjoint variable $(\mathbf{v}, q)$, then integrate by parts, add them together to make (ex-adj-gfld) appear for cancellation, obtain:

$$\boxed{\begin{aligned} &\int_\Omega [\nabla_{\mathbf{u}}J_\Omega(\cdot) - \nabla\cdot(\nabla_{\nabla\mathbf{u}}J_\Omega(\cdot))]\cdot\mathbf{u}'(\mathbf{x};V) + D_pJ_\Omega(\cdot)p'(\mathbf{x};V)\mathrm{d}\mathbf{x} \\ &+ \int_\Gamma [-\nabla_{\mathbf{u}}\mathbf{Q}(\cdot)\mathbf{v}_{\rm bc} + \nabla_{\nabla\mathbf{u}}J_\Omega(\cdot)\cdot\mathbf{n} + \nabla_{\mathbf{u}}J_\Gamma(\cdot)]\cdot\mathbf{u}'(\mathbf{x};V)\mathrm{d}\Gamma \\ &+ \int_\Gamma -\mathbf{v}^\top D_{\Delta\mathbf{u}}\mathbf{P}(\cdot)\partial_{\mathbf{n}}\mathbf{u}'(\mathbf{x};V) + p'(\mathbf{x};V)\mathbf{n}^\top\nabla_{\nabla p}\mathbf{P}(\cdot)\mathbf{v}\mathrm{d}\Gamma = 0. \end{aligned}}$$

1st-order shape derivatives of (gfld)-constrained (cost-gfld)

- Use Theorems 1, 2, obtain:

$$
\begin{aligned}
& dJ(\mathbf{u}, p, \Omega; V) \\
= & \int_\Omega J_\Omega(\cdot; V) + \nabla \cdot (J_\Omega(\cdot) V(0)) \mathrm{d}\mathbf{x} \\
& + \int_\Gamma J'_\Gamma(\cdot; V) + \nabla(J_\Gamma(\cdot)) \cdot V(0) + J_\Gamma(\cdot) \left(\nabla \cdot V(0) - DV(0)\mathbf{n} \cdot \mathbf{n}\right) \mathrm{d}\Gamma \\
= & \int_\Omega J'_\Omega(\cdot; V) \mathrm{d}\mathbf{x} + \int_\Gamma J_\Omega(\cdot) V(0) \cdot \mathbf{n} \mathrm{d}\Gamma \\
& + \int_\Gamma J'_\Gamma(\cdot; V) + \left[\partial_\mathbf{n}(J_\Gamma(\cdot)) + H J_\Gamma(\cdot)\right] V(0) \cdot \mathbf{n} \mathrm{d}\Gamma.
\end{aligned}
$$

- Expand these explicitly, integrate by parts any terms of the forms $\int_\Omega \ldots \cdot \{\nabla \mathbf{u}', \Delta \mathbf{u}', \nabla p'\}(\mathbf{x}; V) \mathrm{d}\mathbf{x}$.
- Cancel all the terms of the form $\int_\Omega \ldots \cdot \{\mathbf{u}', p'\}(\mathbf{x}; V) \mathrm{d}\mathbf{x}$ by the last formula in the previous frame.

1st-order shape derivatives of (gfld)-constrained (cost-gfld)

$$
\begin{aligned}
dJ(\mathbf{u}, p, \Omega; V) = & \int_\Omega \nabla \cdot (J_\Omega(\cdot) V(0)) \,\mathrm{d}\mathbf{x} \\
& + \int_\Gamma \nabla_{\nabla \mathbf{u}} J_\Gamma(\cdot) : \nabla \mathbf{u}'(\mathbf{x}; V) + \partial_p J_\Gamma(\cdot) p'(\mathbf{x}; V) + \nabla_{\mathbf{n}} J_\Gamma(\cdot) \cdot \mathbf{n}'(\mathbf{x}; V) \\
& \qquad + \nabla_{\mathbf{t}} J_\Gamma(\cdot) : \mathbf{t}'(\mathbf{x}; V) + \nabla \left(J_\Gamma(\cdot) \right) \cdot V(0) \\
& \qquad + J_\Gamma(\cdot) \left(\nabla \cdot V(0) - DV(0)\mathbf{n} \cdot \mathbf{n} \right) + \left(\nabla_{\mathbf{u}} \mathbf{Q}(\cdot) \mathbf{v}_{\mathrm{bc}} \right) \cdot \mathbf{u}'(\mathbf{x}; V) \\
& \qquad + \mathbf{v}^\top D_{\Delta \mathbf{u}} \mathbf{P}(\cdot) \partial_{\mathbf{n}} \mathbf{u}'(\mathbf{x}; V) - p'(\mathbf{x}; V) \mathbf{n}^\top \nabla_{\nabla p} \mathbf{P}(\cdot) \mathbf{v} \,\mathrm{d}\Gamma \\
= & \int_\Gamma J_\Omega(\cdot) V(0) \cdot \mathbf{n} + \nabla_{\nabla \mathbf{u}} J_\Gamma(\cdot) : \nabla \mathbf{u}'(\mathbf{x}; V) + \partial_p J_\Gamma(\cdot) p'(\mathbf{x}; V) \\
& \qquad + \nabla_{\mathbf{n}} J_\Gamma(\cdot) \cdot \mathbf{n}'(\mathbf{x}; V) + \nabla_{\mathbf{t}} J_\Gamma(\cdot) : \mathbf{t}'(\mathbf{x}; V) \\
& \qquad + \partial_{\mathbf{n}} \left(J_\Gamma(\cdot) \right) V(0) \cdot \mathbf{n} + H J_\Gamma(\cdot) V(0) \cdot \mathbf{n} \\
& \qquad + \left(\nabla_{\mathbf{u}} \mathbf{Q}(\cdot) \mathbf{v}_{\mathrm{bc}} \right) \cdot \mathbf{u}'(\mathbf{x}; V) + \mathbf{v}^\top D_{\Delta \mathbf{u}} \mathbf{P}(\cdot) \partial_{\mathbf{n}} \mathbf{u}'(\mathbf{x}; V) \\
& \qquad - p'(\mathbf{x}; V) \mathbf{n}^\top \nabla_{\nabla p} \mathbf{P}(\cdot) \mathbf{v} \,\mathrm{d}\Gamma.
\end{aligned}
$$

To eliminate $\{\mathbf{u}', \nabla \mathbf{u}', \partial_{\mathbf{n}} \mathbf{u}', p'\}(\mathbf{x}; V)$, need explicit formulas of $\mathbf{Q}(\cdot)$.

- Adjoint PDEs of (iNS):

$$\boxed{\begin{cases} \mathbf{v}_t + \nu\Delta\mathbf{v} - \nabla\mathbf{u}\mathbf{v} + (\mathbf{u}\cdot\nabla)\mathbf{v} - \nabla q = -\gamma k_\delta \left(\left(p + \frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right) \text{ in } [0,T]\times\Omega, \\ -\nabla\cdot\mathbf{v} = \gamma k_\delta \mathbf{u}\cdot\mathbf{n} \text{ in } [0,T]\times\Omega, \\ \mathbf{v}(T,\cdot) = \mathbf{0} \text{ in } \Omega, \\ \mathbf{v} = \mathbf{0} \text{ on } [0,T]\times(\Gamma_{\mathrm{in}}\cup\Gamma_{\mathrm{wall}}), \\ (\mathbf{u}\cdot\mathbf{n})\mathbf{v} + \nu\partial_{\mathbf{n}}\mathbf{v} - q\mathbf{n} = (1-\gamma)(\mathbf{u}\cdot\mathbf{n} - \overline{u})\mathbf{n} \text{ on } [0,T]\times\Gamma_{\mathrm{out}}. \end{cases}} \tag{adj-iNS}$$

- Assume: $\Gamma_{\mathrm{in}}^\delta$ & $\Gamma_{\mathrm{out}}^\delta$ are fixed, thus $V = \mathbf{0}$ in $[0,T]\times(\Gamma_{\mathrm{in}}^\delta\cup\Gamma_{\mathrm{out}}^\delta)$.
- The 1st-order shape derivative of (iNS)-constrained ($J_{12}^{\delta,\gamma}$):

$$dJ_{12}^{\delta,\gamma}(\mathbf{u},p,\Omega;V) = \int_0^T\int_{\Gamma_{\mathrm{wall}}} \nu\partial_{\mathbf{n}}\mathbf{u}\cdot\partial_{\mathbf{n}}\mathbf{v}V(0)\cdot\mathbf{n}\,\mathrm{d}\Gamma\mathrm{d}t. \tag{dJ}$$

Smagorinsky turbulence models with mixed boundary conditions:

$$
\begin{cases}
\mathbf{w}_t - \nabla \cdot ((2\nu + \nu_t)\varepsilon(\mathbf{w})) + (\mathbf{w} \cdot \nabla)\mathbf{w} + \nabla r = \mathbf{f} & \text{in } (0, T] \times \Omega, \\
\nabla \cdot \mathbf{w} = 0 & \text{in } [0, T] \times \Omega, \\
\mathbf{w}(0, \cdot) = \mathbf{w}_0 & \text{in } \Omega, \\
\mathbf{w} = \mathbf{f}_{\mathrm{in}} & \text{on } [0, T] \times \Gamma_{\mathrm{in}}, \\
\mathbf{w} = \mathbf{0} & \text{on } [0, T] \times \Gamma_{\mathrm{wall}}, \\
-\nu \partial_{\mathbf{n}} \mathbf{w} + r\mathbf{n} = \mathbf{0} & \text{on } [0, T] \times \Gamma_{\mathrm{out}},
\end{cases}
\tag{Smagorinsky}
$$

where $\nu_t := c_S \delta^2 \|\varepsilon(\mathbf{w})\|_{\mathrm{F}}$ for a constant $c_S > 0$, &

$$
\varepsilon(\mathbf{w}) := \frac{1}{2}(\nabla \mathbf{w} + (\nabla \mathbf{w})^\top).
$$

k-ϵ turbulence model, where $Q_T := (0, T) \times \Omega$:

$$\boxed{\begin{cases} \overline{\mathbf{u}}_t + (\overline{\mathbf{u}} \cdot \nabla)\overline{\mathbf{u}} - \nabla \cdot \Big((\nu + \nu_t)(\nabla \overline{\mathbf{u}} + \nabla \overline{\mathbf{u}}^\top) \Big) + \nabla \left(\overline{p} + \dfrac{2}{3} k \right) = \overline{\mathbf{f}} & \text{in } Q_T, \\ \nabla \cdot \overline{\mathbf{u}} = 0 & \text{in } Q_T, \\ k_t + (\overline{\mathbf{u}} \cdot \nabla) k - \nabla \cdot (\nu_t \nabla k) - \dfrac{c_\mu}{2} \dfrac{k^2}{\epsilon} \|\nabla \overline{\mathbf{u}} + (\nabla \overline{\mathbf{u}})^\top\|_{\mathrm{F}}^2 + \epsilon = 0 & \text{in } Q_T, \\ \epsilon_t + (\overline{\mathbf{u}} \cdot \nabla)\epsilon - \nabla \cdot \left(\dfrac{c_\epsilon}{c_\mu} \nu_t \nabla \epsilon \right) - \dfrac{c_1}{2} k \|\nabla \overline{\mathbf{u}} + (\nabla \overline{\mathbf{u}})^\top\|_{\mathrm{F}}^2 + c_2 \dfrac{\epsilon^2}{k} = 0 & \text{in } Q_T, \end{cases}} \tag{k-ϵ}$$

- Adjoint of initial conditions (adj-ICs) of k-ϵ: done.
- Adjoint of boundary conditions (adj-BCs) of k-ϵ: in processing ...
  $\rightarrow$ *wall laws & adjoint wall laws*.

Adjoint of $(k\text{-}\epsilon)$

$$
\begin{cases}
\mathbf{v}_t + \left(\nu + c_\mu \dfrac{k^2}{\epsilon}\right)(\nabla(\nabla\cdot\mathbf{v}) + \Delta\mathbf{v}) + 2c_\mu\varepsilon(\mathbf{v})\nabla\left(\dfrac{k^2}{\epsilon}\right) + \nabla\bar{\mathbf{u}}\mathbf{v} + (\bar{\mathbf{u}}\cdot\nabla)\mathbf{v} - \nabla q \\
\quad = -\partial_{\bar{\mathbf{u}}} J_\Omega + r\nabla k + 4c_\mu\dfrac{k^2}{\epsilon}\varepsilon(\bar{\mathbf{u}})\nabla r + 4c_\mu r\varepsilon(\bar{\mathbf{u}})\nabla\left(\dfrac{k^2}{\epsilon}\right) + 2c_\mu r\dfrac{k^2}{\epsilon}\Delta\bar{\mathbf{u}} \\
\qquad + 2c_\mu\nabla(\nabla\cdot\bar{\mathbf{u}}) + \eta\nabla\epsilon + 4c_1 k\varepsilon(\bar{\mathbf{u}})\nabla\eta + 2c_1\eta\varepsilon(\bar{\mathbf{u}})\nabla k \\
\qquad + 2c_1\eta k(\Delta\bar{\mathbf{u}} + \nabla(\nabla\cdot\bar{\mathbf{u}})) \text{ in } \Omega, \\
\nabla\cdot\mathbf{v} = -\partial_{\bar{p}} J_\Omega \text{ in } \Omega, \\
r_t + c_\mu\dfrac{k^2}{\epsilon}\Delta r + \nabla r\cdot\bar{\mathbf{u}} - 2c_\mu\dfrac{k}{\epsilon}\nabla r\cdot\nabla k + c_\mu\nabla\left(\dfrac{k^2}{\epsilon}\right)\cdot\nabla r \\
\quad = 4c_\mu\dfrac{k}{\epsilon}\varepsilon(\bar{\mathbf{u}}) : \nabla\mathbf{v} - \dfrac{2}{3}\nabla\cdot\mathbf{v} - c_\mu r\dfrac{k}{\epsilon}\|\nabla\bar{\mathbf{u}} + \nabla\bar{\mathbf{u}}^\top\|^2 + 2c_\epsilon\dfrac{k}{\epsilon}\nabla\eta\cdot\nabla\epsilon \\
\qquad - \dfrac{c_1}{2}\eta\|\nabla\bar{\mathbf{u}} + \nabla\bar{\mathbf{u}}^\top\|^2 - c_2\eta\dfrac{\epsilon^2}{k^2} \text{ in } \Omega, \\
\eta_t + c_\epsilon\dfrac{k^2}{\epsilon}\Delta\eta + \nabla\eta\cdot\bar{\mathbf{u}} + c_\epsilon\dfrac{k^2}{\epsilon^2}\nabla\eta\cdot\nabla\epsilon + c_\epsilon\nabla\left(\dfrac{k^2}{\epsilon}\right)\cdot\nabla\eta \\
\quad = -2c_\mu\dfrac{k^2}{\epsilon^2}\varepsilon(\bar{\mathbf{u}}) : \nabla\mathbf{v} + c_\mu\dfrac{k^2}{\epsilon^2}\nabla r\cdot\nabla k + \dfrac{c_\mu}{2}r\dfrac{k^2}{\epsilon^2}\|\nabla\bar{\mathbf{u}} + \nabla\bar{\mathbf{u}}^\top\|^2 + r + 2c_2\eta\dfrac{\epsilon}{k} \text{ in } \Omega.
\end{cases}
\tag{adj-k-ϵ}
$$

Compute 1st-order shape derivatives

How to compute the 1st-order shape derivative of a PDEs-constrained shape functional via (continuous) adjoint approach:

- Derive adjoint of the PDEs via integration by parts;
- Derive PDEs for the local shape derivative(s) of solution(s) of that PDEs;
- Derive the weak formulation of the PDEs in Step 2 with adjoint variable(s) as test function(s)
  $\rightarrow$ Simplify it by the adjoint PDEs in Step 1;
- Use the standard formulas for domain &/or boundary integrals to calculate the "raw" 1st-order shape derivative;
- Simplify it by the equality obtained at the end of Step 3
  $\rightarrow$ Eliminate local shape derivative(s) in domain integrals of the "raw" 1st-order shape derivative.

Output. A "cooked"/implementable 1st-order shape derivative.

Progress

- Derived adjoint PDEs for stationary + instationary NSEs, & k-ϵ turbulence models.
- Computed 1st-order shape derivative for (general) stationary NSEs & (specific) instationary NSEs via continuous adjoint approach (not yet for k-ϵ due to *wall laws* & its adjoint).
- Basic OpenFOAM.

Software development & numerics

- Topology Optimization: compute *topological derivatives*.
- Establish *Finite Volume schemes* for the SOPs considered.
- Dive in OpenFOAM to know available PDEs solvers & boundary conditions.
- Derive formally the adjoint equations for OpenFOAM's PDEs & OpenFOAM's boundary conditions.

- Auer, Naomi; Hintermüller, Michael; Knall, Karl (2020). *Benchmark case for optimal shape design of air ducts in combustion engines*. ROMSOC D5.1, version 3.0.
- Delfour, M. C.; J.-P. Zolésio (2011). *Shapes & geometries. Second. Vol. 22. Advances in Design & Control. Metrics, analysis, differential calculus, & optimization*. Society for Industrial & Applied Mathematics (SIAM), Philadelphia, PA, pp. xxiv+622.
- Maz'ya, V.; Rossmann, J (2009). "Mixed boundary value problems for the stationary Navier-Stokes system in polyhedral domains". *Arch. Ration. Mech. Anal.* 194, no. 2, 669–712.
- Mohammadi, B.; O. Pironneau (1994). *Analysis of the k-epsilon turbulence model*. RAM: Research in Applied Mathematics. Masson, Paris; John Wiley & Sons, Ltd., Chichester, pp. xiv+196.

- Othmer, C (2008). "A continuous adjoint formulation for the computation of topological & surface sensitivities of ducted flows". In: *Internat. J. Numer. Methods Fluids* 58.8, pp. 861–877.
- Sokołowski, Jan; Jean-Paul Zolésio (1992). *Introduction to shape optimization*. Vol. 16. Springer Series in Computational Mathematics. Shape sensitivity analysis. Springer-Verlag, Berlin, pp. ii+250.
- Temam, Roger (2000). *Navier-Stokes equations. Theory & numerical analysis*. Studies in Mathematics & its Applications, Vol. 2. AMS Chelsea Publishing, p. 408.
- Tsai, Tai-Peng (2018). *Lectures on Navier-Stokes equations*. Vol. 192. Graduate Studies in Mathematics. AMS, Providence, RI, pp. xii+224.