Shape optimization governed by generalized Navier-Stokes equations

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Outline

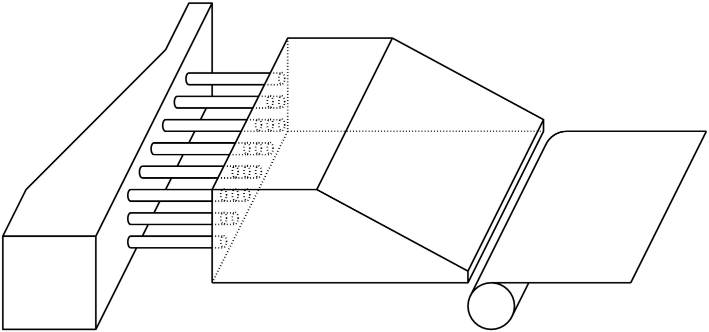
Motivation: Paper making industry

Figure: Paper making machine

Goal of mathematical modelling:

- derive sufficiently accurate model
- increase quality and production rate

Wet section of paper making machine



1. Mixture of water and wood fibres enters the **dividing header**
2. Limited amount of mixture is suck off through **recirculation**
3. The rest flows out through **pipes** into **equalizing chamber**
4. In **slice channel** the speed is increased
5. Mixture is put on a **wire**

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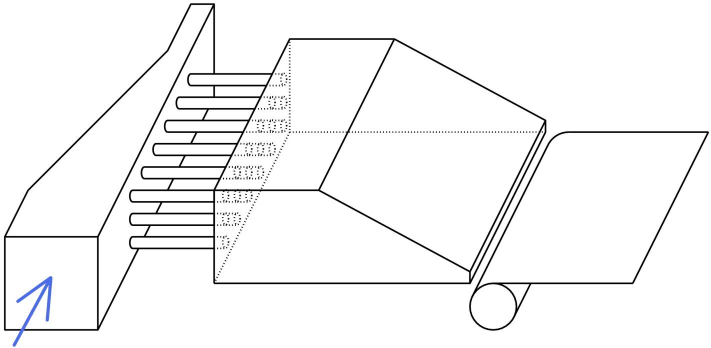

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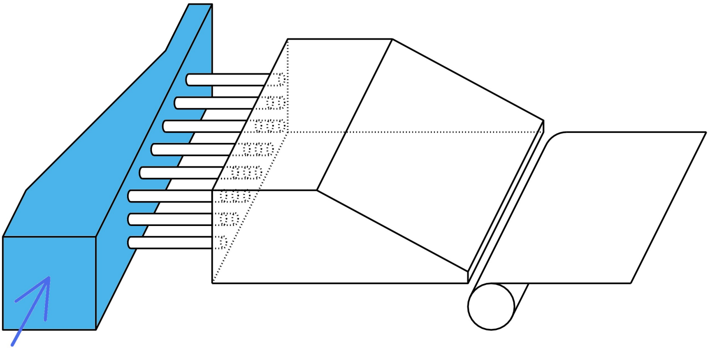

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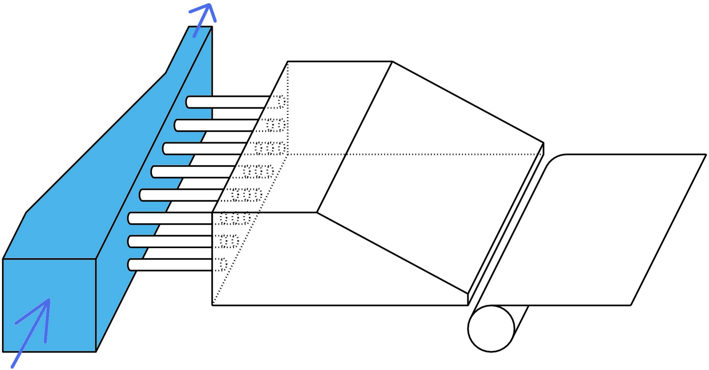

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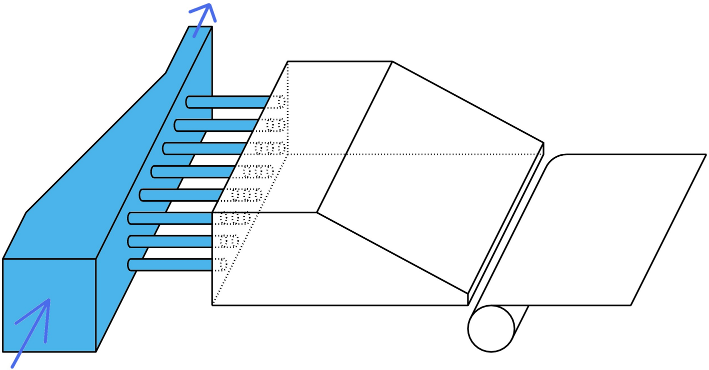

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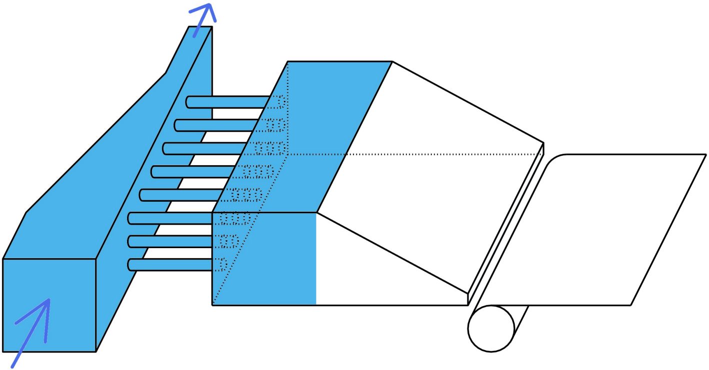

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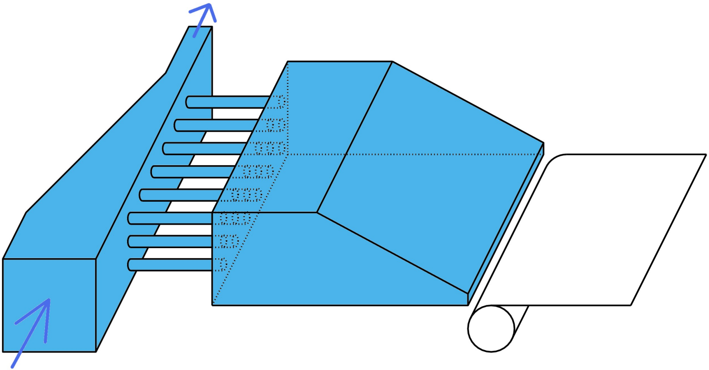

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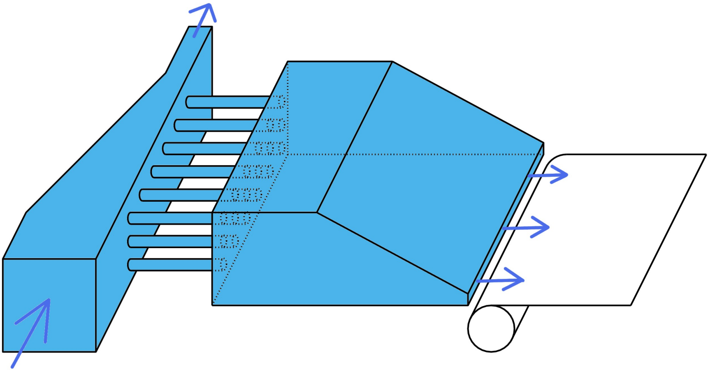

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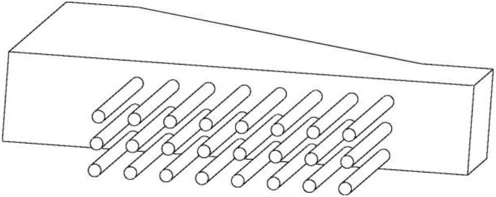
Dividing header



Flow in the header has great impact on

- basis weight of produced paper
- fibre orientation

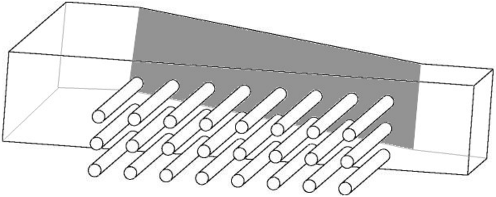
Optimization goal

- to control the outlet velocity in pipes:

$$\min \int_{\Gamma_{out}} \left| v_{\nu} - v_{opt} \right|$$

- control variable: shape of back wall

Dividing header



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Previous results

- Hämäläinen, Mäkinen, Tarvainen [1993, 1999] - model and numerical solution
- S., H., M. [2005] - existence result for velocity-based formulation

I. Analysis of the continuous problem

Description of geometry

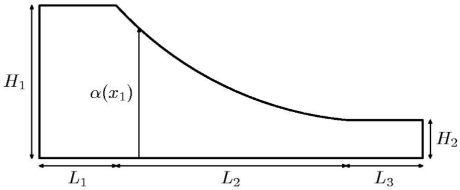


Figure: Geometry of $\Omega(\alpha)$

Admissible domains

$$\Omega(\alpha) := \left\{ x \in \mathbb{R}^2;\ 0 < x_1 < L,\ 0 < x_2 < \alpha(x_1) \right\},$$

where α is an element of

$$\mathcal{U}_{ad} := \{\alpha \in C^{0,1}([0,L]);\ \alpha|_{[0,L_1]} = H_1,\ \alpha|_{[L_1+L_2,L]} = H_2,\ \alpha_{min} \leq \alpha \leq \alpha_{max},\ |\alpha'| \leq \gamma\}$$

Equations of motion

Fluid flow characteristics

- continuum
- stationary model for averaged velocity and pressure
- simple turbulence model

Flow equations

$$
\begin{aligned}
-\operatorname{div}\mathbb{T} + \rho\operatorname{div}(\mathbf{v}\otimes\mathbf{v}) &= \mathbf{0} \\
\operatorname{div}\mathbf{v} &= 0
\end{aligned}
$$

Stress tensor $\quad \mathbb{T} = -p\mathbb{I} + \mu\mathbb{D}(\mathbf{v})$

Viscosity $\quad \mu(x, |\mathbb{D}(\mathbf{v})|^2) = \mu_0 + \rho l_{m,\alpha}^2(x)|\mathbb{D}(\mathbf{v})|$

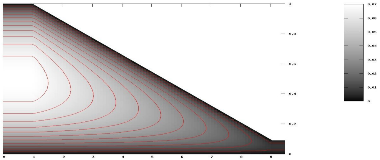
Choice of $l_{m,\alpha}$:

- $l_{m,\alpha} = 0$: Navier-Stokes
- $l_{m,\alpha} = \mathit{const.} > 0$: non-Newtonian fluid
- our model: generalization - geometry dependent function

Mixing length $l_{m,\alpha}$ represents an algebraic turbulence model:

$$l_{m,\alpha}(x) = \frac{1}{2}\alpha(x_1)\left[0.14 - 0.08\left(1 - \frac{2d_\alpha(x)}{\alpha(x_1)}\right)^2 - 0.06\left(1 - \frac{2d_\alpha(x)}{\alpha(x_1)}\right)^4\right],$$

$$d_\alpha(x) = \min\left\{x_2, \alpha(x_1) - x_2\right\}, x \in \Omega(\alpha).$$



Properties:

- $l_{m,\alpha} \in C(\overline{\Omega(\alpha)})$;
- $l_{m,\alpha} \geq 0$ in $\overline{\Omega(\alpha)}$, $l_{m,\alpha} > 0$ in $\Omega(\alpha)$;
- $l_{m,\alpha} \approx \mathrm{dist}_{\partial\Omega(\alpha)\setminus\Gamma_D}$

Boundary conditions

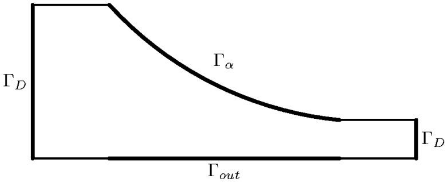


Figure: Boundary segments of $\partial\Omega(\alpha)$

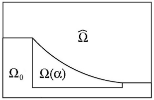
$$\begin{aligned} \mathbf{v} &= \mathbf{v}_D && \text{on } \Gamma_D, \\ \mathbf{v} &= \mathbf{0} && \text{on } \partial\Omega(\alpha) \setminus (\Gamma_D \cup \Gamma_{out}), \end{aligned}$$

On Γ_{out} we use a nonlinear outflow b.c. which replaces the system of pipes:

$$\begin{aligned} v_1 &= 0, \\ \mathbb{T}_{22} &= -\sigma |v_2| v_2, \ \sigma > 0. \end{aligned}$$

Weak formulation

We construct $\mathbf{v}_0 \in W^{1,3}(\widehat{\Omega})$ which extends the Dirichlet b.c. and is independent of α.



Weak formulation (P(α))

Find $(\mathbf{v}, p) \in W(\alpha) \times L(\alpha)$ such that $\mathbf{v} - \mathbf{v}_0 \in W_0(\alpha)$,

$$2\mu_0 \int_{\Omega(\alpha)} \mathbb{D}(\mathbf{v}) : \mathbb{D}(\varphi) + 2\rho \int_{\Omega(\alpha)} l_{m,\alpha}^2 |\mathbb{D}(\mathbf{v})| \mathbb{D}(\mathbf{v}) : \mathbb{D}(\varphi)$$

$$+ \rho \int_{\Omega(\alpha)} v_j \frac{\partial v_i}{\partial x_j} \varphi_i + \sigma \int_{\Gamma_{out}} |v_2| v_2 \varphi_2 - \int_{\Omega(\alpha)} p \operatorname{div} \varphi = 0,$$

$$\int_{\Omega(\alpha)} \psi \operatorname{div} \mathbf{v} = 0$$

for all $\varphi \in W_0(\alpha)$, $\psi \in L(\alpha)$.

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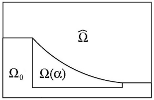

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Choice of function spaces

$$W(\alpha) := \overline{\mathcal{V}(\alpha)}^{\|\cdot\|_\alpha}$$

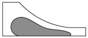
$$W_0(\alpha) := \overline{\mathcal{V}_0(\alpha)}^{\|\cdot\|_\alpha}$$

$$L(\alpha) := L^{\frac{3}{2}}(\Omega(\alpha))$$

Norm:

$$\|\mathbf{w}\|_\alpha := \|\mathbf{w}\|_{1,2,\Omega(\alpha)} + \| l_{m,\alpha}^{2/3} \mathbb{D}(\mathbf{w}) \|_{3,\Omega(\alpha)} + \| \operatorname{div} \mathbf{w} \|_{3,\Omega(\alpha)}$$

$$\mathcal{V}(\alpha) := \left(C^\infty(\overline{\Omega(\alpha)}) \right)^2$$

$$\mathcal{V}_0(\alpha) := \left\{ \mathbf{w} \in \mathcal{V}(\alpha);\ \operatorname{supp} \mathbf{w} = \right.$$  $$\left. \right\}$$

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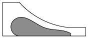
$$\mathcal{V}_0(\alpha) := \left\{ \mathbf{w} \in \mathcal{V}(\alpha); \;\; \operatorname{supp} \mathbf{w} = \right.$$  $$\left. \right\}$$

Choice of function spaces - cont.

Alternative definition:

$$\widehat{W}(\alpha) := \left\{ \mathbf{w} \in \left(W^{1,2}(\Omega(\alpha))\right)^2;\ \|\mathbf{w}\|_\alpha < \infty \right\},$$

$$\widehat{W}_0(\alpha) := \left\{ \mathbf{w} \in \widehat{W}(\alpha);\ \ \operatorname{Tr} \mathbf{w}|_{\partial\Omega(\alpha)\setminus\Gamma_{out}} = \mathbf{0},\ \ \operatorname{Tr} w_1|_{\Gamma_{out}} = 0 \right\}.$$

Properties:

- $\left(W^{1,3}(\Omega(\alpha))\right)^2 \hookrightarrow W(\alpha) \hookrightarrow \widehat{W}(\alpha) \hookrightarrow \left(W^{1,2}(\Omega(\alpha))\right)^2$
- $W(\alpha), \widehat{W}(\alpha)$ are separable and reflexive
- $W(\alpha) = \widehat{W}(\alpha)$
- $W_0(\alpha) \stackrel{?}{=} \widehat{W}_0(\alpha)$

For the weak formulation we need density of $\mathcal{V}_0(\alpha) \Rightarrow$ use $W_0(\alpha)$.

Existence of solutions to $(P(\alpha))$

1. **Aproximate model ($\mathbf{P}^\varepsilon(\alpha)$)**

$$\begin{aligned} -\operatorname{div}\mathbb{T} + \rho\operatorname{div}(\mathbf{v}^\varepsilon \otimes \mathbf{v}^\varepsilon) &= -\frac{\rho}{2}(\operatorname{div}\mathbf{v}^\varepsilon)(\mathbf{v}^\varepsilon - \mathbf{v}_0) \\ \operatorname{div}\mathbf{v}^\varepsilon &= -\varepsilon|p^\varepsilon|^{-\frac{1}{2}}p^\varepsilon \end{aligned}$$

2. **Apriori estimate for ($\mathbf{P}^\varepsilon(\alpha)$)**
   Inserting $\varphi := \mathbf{v}^\varepsilon - \mathbf{v}_0$, $\psi := p^\varepsilon$ we obtain for $\sigma > \frac{\rho}{2}$:

$$\|\mathbb{D}(\mathbf{v}^\varepsilon)\|_2^2 + \|I_{m,\alpha}^{2/3}\mathbb{D}(\mathbf{v}^\varepsilon)\|_3^3 + \|v_2^\varepsilon\|_{3,\Gamma_{out}}^3 + \varepsilon\|p^\varepsilon\|_{\frac{3}{2}}^{\frac{3}{2}} \leq C_E,$$

   where C_E is independent of α. Restriction is due to convective term and nonlinear b.c.

3. **Existence of solution to ($\mathbf{P}^\varepsilon(\alpha)$) - Galerkin method**

4. **Uniform estimate of pressure (with resp. to ε)**
It holds: For every $f \in L^3(\Omega(\alpha))$ there exists $\mathbf{w} \in W_0(\alpha)$:

$$\operatorname{div} \mathbf{w} = f \text{ v } \Omega(\alpha)$$
$$\|\mathbf{w}\|_\alpha \leq C\|f\|_3$$

where $C > 0$ is independent of α.

$$\Rightarrow \inf_{q \in L(\alpha)} \sup_{\mathbf{w} \in W(\alpha)} \frac{\int_{\Omega(\alpha)} q \operatorname{div} \mathbf{w}}{\|q\|_{\frac{3}{2}} \|\mathbf{w}\|_\alpha} \geq C$$

$$\Rightarrow \|p^\varepsilon\|_{\frac{3}{2}} \leq C$$

5. **Limit passage $\varepsilon \to 0+$:** Using that

$$\mathbf{v}^\varepsilon \rightharpoonup \mathbf{v} \qquad \text{in } W^{1,2}(\Omega(\alpha)),$$
$$p^\varepsilon \rightharpoonup p \qquad \text{in } L^{3/2}(\Omega(\alpha)),$$

we can proceed:

$$\int_{\Omega(\alpha)} \mathbb{D}(\mathbf{v}^\varepsilon) : \mathbb{D}(\varphi) \to \int_{\Omega(\alpha)} \mathbb{D}(\mathbf{v}) : \mathbb{D}(\varphi),$$
$$\int_{\Omega(\alpha)} v_j^\varepsilon \frac{\partial v_i^\varepsilon}{\partial x_j} \varphi_i \to \int_{\Omega(\alpha)} v_j \frac{\partial v_i}{\partial x_j} \varphi_i,$$
$$\int_{\Gamma_{out}} |v_2^\varepsilon| v_2^\varepsilon \varphi_2 \to \int_{\Gamma_{out}} |v_2| v_2 \varphi_2,$$
$$\int_{\Omega(\alpha)} p^\varepsilon \operatorname{div} \varphi \to \int_{\Omega(\alpha)} p \operatorname{div} \varphi.$$

The difficult weighted term is handled using monotonicity and Minty's trick:

$$\int_{\Omega(\alpha)} l_{m,\alpha}^2 |\mathbb{D}(\mathbf{v}^\varepsilon)| \mathbb{D}(\mathbf{v}^\varepsilon) : \mathbb{D}(\varphi) \to \int_{\Omega(\alpha)} l_{m,\alpha}^2 |\mathbb{D}(\mathbf{v})| \mathbb{D}(\mathbf{v}) : \mathbb{D}(\varphi)$$

Existence of solution to (P(α)) - summary

Theorem

Let $\sigma > \frac{\rho}{2}$. Then for every $\alpha \in \mathcal{U}_{ad}$:

- *there exists a solution* $(\mathbf{v}, p)$,
- *for every solution* $(\mathbf{v}, p)$ *the following estimate holds:*

$$\|\mathbb{D}(\mathbf{v})\|_2^2 + \|I_{m,\alpha}^{2/3}\mathbb{D}(\mathbf{v})\|_3^3 + \|v_2\|_{3,\Gamma_{out}}^3 + \|p\|_{\frac{3}{2}}^{\frac{3}{2}} \le C_E,$$

- *pressure* p *is determined uniquely by velocity* $\mathbf{v}$,
- *for* $\|\nabla \mathbf{v}_0\|_3 < C$ *there is exactly one solution.*

Shape optimization problem

$$\mathcal{G} := \{(\alpha, \mathbf{v}, p);\ \alpha \in \mathcal{U}_{ad},\ (\mathbf{v}, p) \text{ is a solution of } (P(\alpha))\}$$

Formulation

- Let $v_{opt} \in L^2(\Gamma_{out})$. Define the cost function $J : \mathcal{G} \to \mathbb{R}$:

$$J(\alpha, \mathbf{v}, p) := \int_{\Gamma_{out}} |v_2 - v_{opt}|^2.$$

- Find $(\alpha^*, \mathbf{v}^*, p^*)$ such that

$$J(\alpha^*, \mathbf{v}^*, p^*) \le J(\alpha, \mathbf{v}, p) \quad \forall (\alpha, \mathbf{v}, p) \in \mathcal{G}. \qquad (\mathbb{P})$$

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Existence of optimal shape

Idea of the proof

Bolzanova-Weierstrass theorem: Continuous function attains its minimum on a compact set.

Questions

1. Is $\mathcal{U}_{ad}$ compact metric space?
2. Is $\alpha \mapsto (\mathbf{v}(\alpha), p(\alpha))$ continuous mapping?

Ad 1.: System $\mathcal{U}_{ad}$ equipped with uniform convergence is compact (Arzelà-Ascoli)

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Ad 2.:

Theorem

Let $\{(\alpha_n, \mathbf{v}(\alpha_n), p(\alpha_n))\}$ *and* $\alpha_n \rightrightarrows \alpha$. *Then there is a subsequence* $\{(\mathbf{v}(\alpha_n), p(\alpha_n))\}$ *and limits* $\mathbf{v}(\alpha) \in \mathbf{v}_0 + \widehat{W}_0(\alpha)$, $p(\alpha) \in L^{3/2}(\Omega(\alpha))$:

$$\begin{aligned} \tilde{\mathbf{v}}(\alpha_n) &\rightharpoonup \tilde{\mathbf{v}}(\alpha) && \text{in } W^{1,2}(\widehat{\Omega}) \\ l_{m,\alpha_n}^{2/3}\mathbb{D}(\tilde{\mathbf{v}}(\alpha_n)) &\rightharpoonup l_{m,\alpha}^{2/3}\mathbb{D}(\tilde{\mathbf{v}}(\alpha)) && \text{in } L^3(\widehat{\Omega}) \\ \tilde{p}(\alpha_n) &\rightharpoonup \tilde{p}(\alpha) && \text{in } L^{3/2}(\widehat{\Omega}). \end{aligned}$$

If $\mathbf{v}(\alpha) \in \mathbf{v}_0 + W_0(\alpha)$, *then* $(\mathbf{v}(\alpha), p(\alpha))$ *is a solution of (P(*α*)).*

Idea of the proof:

1. Choose test functions $\varphi \in W_0(\alpha)$, $\psi \in L(\alpha)$ with compact support $\Rightarrow \varphi \in W_0(\alpha_n)$, $\psi \in L(\alpha_n)$ for n large enough.

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$$\begin{aligned} \tilde{\mathbf{v}}(\alpha_n) &\rightharpoonup \tilde{\mathbf{v}}(\alpha) && \text{in } W^{1,2}(\widehat{\Omega}) \\ I^{2/3}_{m,\alpha_n}\mathbb{D}\left(\tilde{\mathbf{v}}(\alpha_n)\right) &\rightharpoonup I^{2/3}_{m,\alpha}\mathbb{D}\left(\tilde{\mathbf{v}}(\alpha)\right) && \text{in } L^3(\widehat{\Omega}) \\ \tilde{p}(\alpha_n) &\rightharpoonup \tilde{p}(\alpha) && \text{in } L^{3/2}(\widehat{\Omega}). \end{aligned}$$

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2. Pass to the limit in (P(α)).
   The difficult weighted term is handled using strong monotonicity and Vitali's theorem:

$$\int_{\Omega(\alpha_n)} l^2_{m,\alpha_n} |\mathbb{D}(\mathbf{v}(\alpha_n))| \mathbb{D}(\mathbf{v}(\alpha_n)) : \mathbb{D}(\varphi) \to \int_{\Omega(\alpha)} l^2_{m,\alpha} |\mathbb{D}(\mathbf{v})| \mathbb{D}(\mathbf{v}) : \mathbb{D}(\varphi)$$

3. Thanks to the density in $W_0(\alpha)$, (P(α)) holds for all $\boldsymbol{\varphi} \in W_0(\alpha)$, $\psi \in L(\alpha)$.

How to ensure that the limit $\mathbf{v}(\alpha)$ is a solution?

Redefine the state problem allowing solutions from $\mathbf{v}_0 + \widehat{W}_0(\alpha)$.

Augmented state problem $(\widehat{P}(\alpha))$

Find $(\mathbf{v}, p) \in \widehat{W}(\alpha) \times L(\alpha)$ such that $\mathbf{v} - \mathbf{v}_0 \in \widehat{W}_0(\alpha)$, and $(\mathbf{v}, p)$ satisfy the same identity as in $(\mathrm{P}(\alpha))$.

Augmented shape optimization problem $(\widehat{\mathbb{P}})$

Define

$$\widehat{\mathcal{G}} := \left\{(\alpha, \mathbf{v}, p);\ \alpha \in \mathcal{U}_{ad},\ (\mathbf{v}, p) \text{ is a solution of } (\widehat{P}(\alpha))\right\}.$$

Find $(\alpha^*, \mathbf{v}^*, p^*)$ such that

$$J(\alpha^*, \mathbf{v}^*, p^*) \le J(\alpha, \mathbf{v}, p) \quad \forall(\alpha, \mathbf{v}, p) \in \widehat{\mathcal{G}}. \qquad (\widehat{\mathbb{P}})$$

How to ensure that the limit $\mathbf{v}(\alpha)$ is a solution?
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- All results obtained for (P(α)) are valid for ($\widehat{P}(\alpha)$) as well.
- The control-to-state mapping is continuous using ($\widehat{P}(\alpha)$).

Theorem

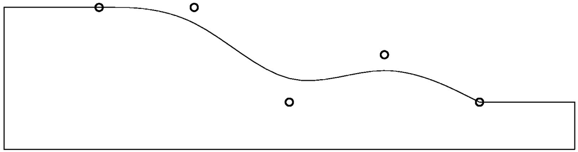
Problem ($\widehat{\mathbb{P}}$) *has a solution.*

II. Analysis of approximate shape optimization problem

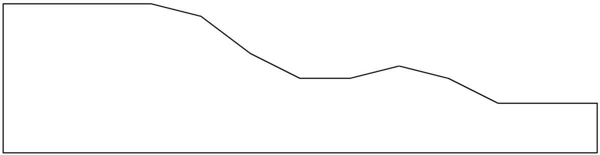
Approximation of the domain $\Omega(\alpha)$:

$$\alpha \in \mathcal{U}_{ad} \mapsto s_{\varkappa} \in \mathcal{U}_{ad}^{\varkappa} \mapsto r_h s_{\varkappa}$$

$\mathcal{U}_{ad}^{\varkappa}$...approximation of $\mathcal{U}_{ad}$ using Bézier functions:



r_h...projection of $\mathcal{U}_{ad}^{\varkappa}$ onto piecewise linear functions.



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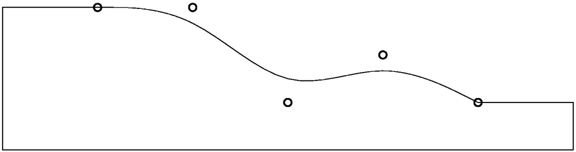

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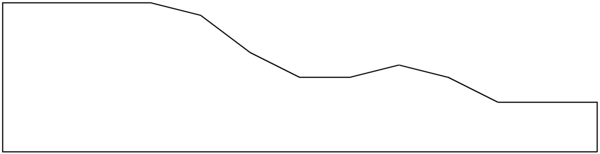

Discrete state problem

- Approximation of function spaces: (W_{0h}, L_h) - MINI element.
- Discrete state problem $(P_h(r_h s_\varkappa))$ - analogy of $(P(\alpha))$ on the spaces W_h, L_h.
- Existence of discrete solution: Under the same assumptions as in the continuous case.
- Stability of (W_{0h}, L_h):

$$\forall \varphi_h \in W_{0h}\ (\psi_h, \operatorname{div} \varphi_h) = 0 \Rightarrow \psi_h \equiv 0.$$

  - pressure is determined uniquely by velocity.
- Boundedness of the pressure and convergence to a solution of the continuous problem: Under the assumption that the discrete inf-sup condition holds.

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Discrete shape optimization problem

- Discrete problem $(\mathbb{P}_{\varkappa h})$ - analogy of $(\mathbb{P})$.
- Existence of optimal discrete shape: Uniformly regular and topologically equivalent triangulations are needed.
- Convergence of solutions of $(\mathbb{P}_{\varkappa h})$ to a solution of $(\widehat{\mathbb{P}})$: Under the assumption that solutions of the state problem are unique and that inf-sup condition holds.

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III. Numerical realization

Numerical realization

State problem

- $\mathbf{a} := (a_1, \ldots, a_n)$: control points of $s_\varkappa$,
- vector of DOFs:

$$\mathbf{v}_h := \mathbf{v}_0 + \sum_{i=0}^{m_1} q_i \boldsymbol{\varphi}_i, \;\; p_h := \sum_{i=1}^{m_2} q_{m_1+i} \psi_i, \;\; \mathbf{q} = \mathbf{q}(\mathbf{a}) \in \mathbb{R}^{m_1+m_2}$$

- discrete state problem $(P_h(r_h s_\varkappa)) \Leftrightarrow \mathbf{R}(\mathbf{a}, \mathbf{q}(\mathbf{a})) = \mathbf{0}$
- linearization: Newton-Raphson method:
  Given $\mathbf{q}_k$, compute $\delta\mathbf{q}_k$:

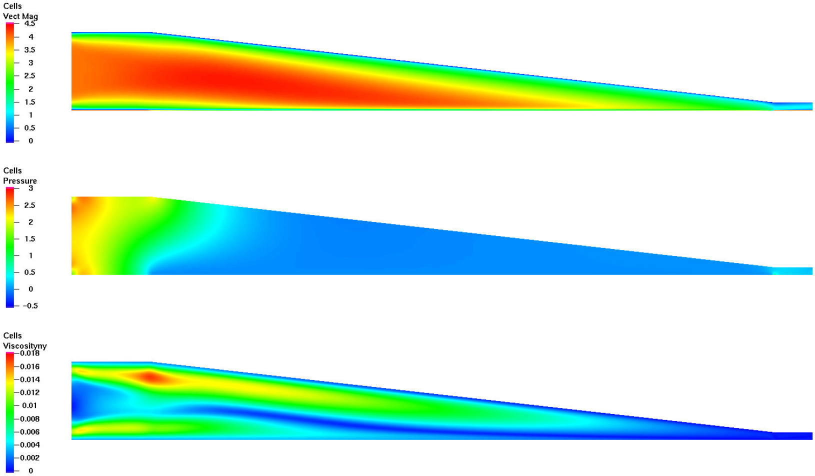
$$\frac{\partial \mathbf{R}(\mathbf{q}_k)}{\partial \mathbf{q}} \delta\mathbf{q}_k = \mathbf{R}(\mathbf{q}_k)$$

  and define $\mathbf{q}_{k+1} := \mathbf{q}_k - \delta\mathbf{q}_k$
- sparse direct solver of linear systems (SuperLU)

Example computation of the state problem

Dimensions: length 9.5m, width 1m

Physical parameters: $\rho = 10^3$, $\mu_0 = 10^{-3}$, $\sigma = 10^3$



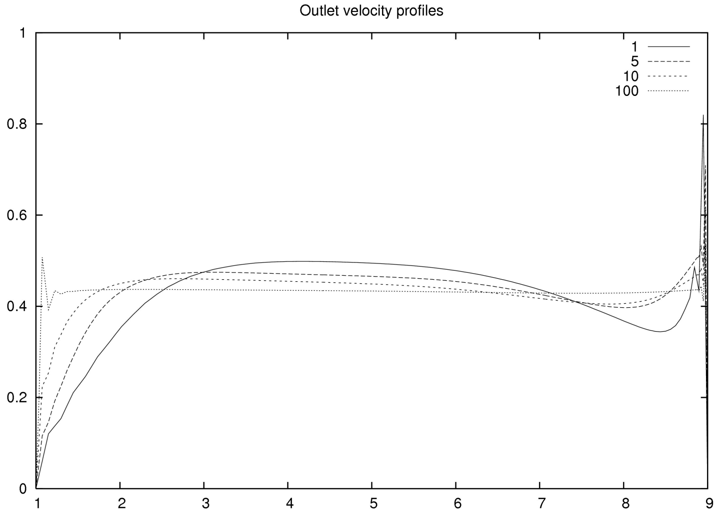


Figure: Outlet velocity profile $v_{2|\Gamma_{out}}$ depending on σ/ρ.

Realization of shape optimization problem

- gradient-based minimization
- adjoint equation:

$$\frac{\mathrm{d}J_h(\mathbf{q}(\mathbf{a}))}{\mathrm{d}a_k} = -\mathbf{p}^{\mathrm{T}}\left(\frac{\partial \mathbf{R}}{\partial a_k}(\mathbf{a}, \mathbf{q}(\mathbf{a}))\right),$$

  where $\mathbf{p}$ is a solution to

$$\left(\frac{\partial \mathbf{R}}{\partial \mathbf{q}}(\mathbf{a}, \mathbf{q}(\mathbf{a}))\right)^{\mathrm{T}} \mathbf{p} = \frac{\partial J_h(}{\partial \mathbf{q}}\mathbf{q}(\mathbf{a}))$$

- derivatives $\frac{\partial \mathbf{R}}{\partial \mathbf{q}}$, $\frac{\partial \mathbf{R}}{\partial \mathbf{a}}$, $\frac{\partial J_h}{\partial \mathbf{q}}$ are calculated using automatic differentiation

Example computation - constant target

Target velocity profile: $v_{ad} = -0.45\ m/s$
Initial geometry: traditional linearly tapered header.

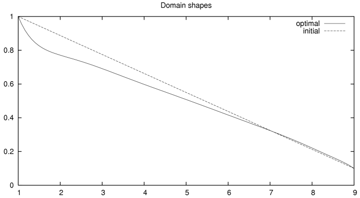


Figure: Initial and optimal shape

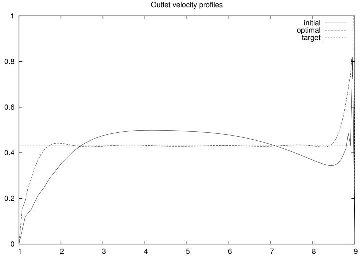
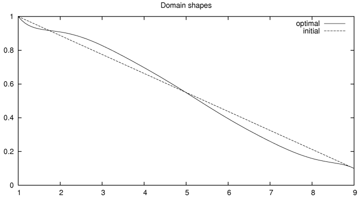


Figure: Initial and optimal velocity profile on Γ_{out}

Example computation - nonconstant target

Target velocity profile: $v_{ad}(x) = -0.65 \sin \frac{\pi}{L2}(x - L_1)\ m/s$
Initial geometry: traditional linearly tapered header.



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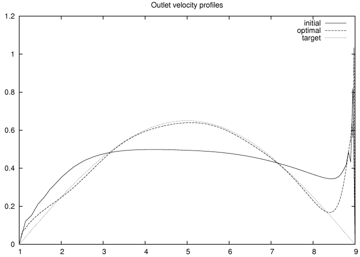

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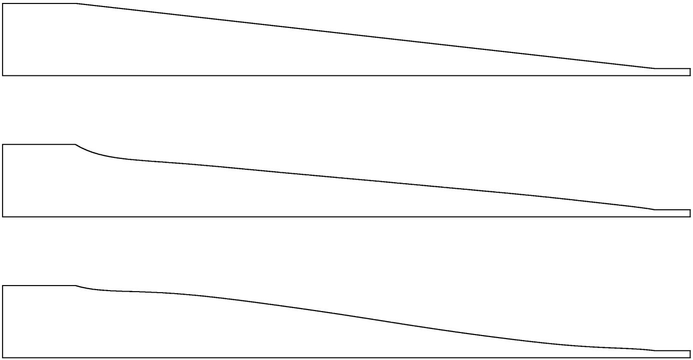

Figure: Geometry - initial, optimized for constant and for nonconstant profile

Summary

Obtained results

- existence of solution to a mixed (velocity-pressure) formulation
  - outflow boundary condition
  - uniqueness of pressure
- existence of solutions to augmented shape optimization problem
- existence and convergence of discrete solutions
  - stability of MINI element
- SW implementation

Thank you for attention.

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