Jan Stebel; Raino Mäkinen; Jukka I. Toivanen

Optimal shape design in a fibre orientation model

Applications of Mathematics, Vol. 52 (2007), No. 5, 391–405

Persistent URL: http://dml.cz/dmlcz/134684

OPTIMAL SHAPE DESIGN IN A FIBRE ORIENTATION MODEL*

Jan Stebel, Praha, Raino A. E. Mäkinen, Jyväskylä,
and Jukka I. Toivanen, Jyväskylä

(Received December 13, 2005, in revised version March 2, 2006)

Abstract. We study a 2D model of the orientation distribution of fibres in a paper machine headbox. The goal is to control the orientation of fibres at the outlet by shape variations. The mathematical formulation leads to an optimization problem with control in coefficients of a linear convection-diffusion equation as the state problem. Existence of solutions both to the state and the optimization problem is analyzed and sensitivity analysis is performed. Further, discretization is done and a numerical example is shown.

Keywords: fibre suspension flow, convection-diffusion equation, optimal control, sensitivity analysis, finite element method, automatic differentiation

MSC 2000: 35J55, 49Q10, 49Q12, 76M10

1. Introduction

A simplified mathematical model describing the orientation of fibres moving through a paper machine headbox slice channel was derived in [12]. The slice channel is a contracting nozzle accelerating the mixture of water and wood fibres to a machine speed. In this paper we continue the study of an optimal control problem formulated in [11]. The goal of the optimization problem is to obtain prescribed fibre orientation distribution at the outlet of the slice channel by changing its shape. For more results on modelling and optimization of a paper machine headbox see e.g. [5], [6], [8].

* This research was supported by the Charles University Grant Agency under Contract 6/2005/R, MSM 0021620839 (MŠMT ČR), and the Academy of Finland, Grant #204741.

The geometry of a planar contracting nozzle (one-dimensional headbox) is described by a Lipschitz continuous function α (see Fig. 1). For simplicity, one-dimensional steady flow $u = (u_1(x_1), 0)$ is assumed. The model further considers the distribution $\psi = \psi(x_1, \varphi)$ of the projected angle φ of the fibre only along the central streamline.

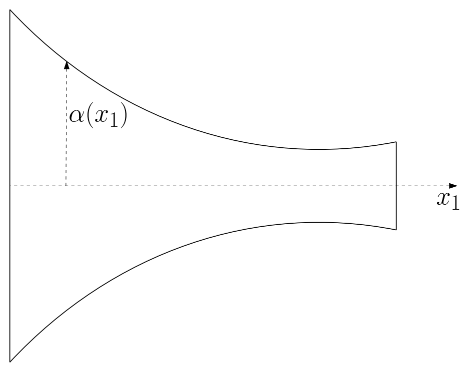

Figure 1. Geometry of the planar contraction.

The distribution ψ is modelled by a linear convection-diffusion equation. This type of problems was analysed e.g. in [9] or [10]. It does not generally possess unique solution, therefore it is desirable to verify that our problem is well posed.

The text is organized as follows. Section 2 deals with existence of a solution to the state problem. Section 3 is devoted to the formulation of an optimal control problem, the existence of its solution, sensitivity analysis and optimality conditions. In Section 4 we describe an approximation of the problem and present a numerical example.

2. Convection-diffusion equation

The probability distribution ψ is given by the solution of the linear convection-diffusion problem in the domain $\Omega = (0,1) \times (-\frac{1}{2}\pi, \frac{1}{2}\pi)$:

$$(\mathrm{P}(\alpha)) \qquad \begin{cases} -\operatorname{div}(\mathcal{A}\nabla\psi) + b_\alpha \cdot \nabla\psi + c_\alpha\psi = 0 & \text{in } \Omega, \\ \psi = \psi_D := \pi^{-1} & \text{on } \Gamma_1, \\ \mathcal{A}\nabla\psi \cdot \nu = 0 & \text{on } \Gamma_2 \cup \Gamma_3. \end{cases}$$

Here $\mathcal{A}$ is a constant positive definite matrix, ν denotes the unit outward normal vector to $\partial\Omega$ and the coefficients b_α, c_α are given by

$$(1) \qquad b_\alpha(x_1, \varphi) = \Big(u_1, -\sin(2\varphi)\frac{\partial u_1}{\partial x_1}\Big), \quad c_\alpha(x_1, \varphi) = -2\cos(2\varphi)\frac{\partial u_1}{\partial x_1}.$$

The symbols Γ_1, Γ_2, Γ_3 denote the following parts of $\partial\Omega$: $\Gamma_1 = \{0\} \times (-\frac{1}{2}\pi, \frac{1}{2}\pi)$, $\Gamma_2 = \{1\} \times (-\frac{1}{2}\pi, \frac{1}{2}\pi)$, $\Gamma_3 = (0,1) \times \{-\frac{1}{2}\pi, \frac{1}{2}\pi\}$.

In order to eliminate the flow field from the model, we assume that the flow is one-dimensional, i.e. $u = (u_1(x_1), 0)$. The continuity of the flow then implies $u_1(x_1) = \beta/\alpha(x_1)$, where $\beta > 0$. Consequently the coefficients of the equation are of the form

$$b_\alpha(x_1,\varphi) = \Big(\frac{\beta}{\alpha(x_1)}, \frac{\beta\alpha'(x_1)}{\alpha^2(x_1)}\sin(2\varphi)\Big), \quad c_\alpha(x_1,\varphi) = \frac{2\beta\alpha'(x_1)}{\alpha^2(x_1)}\cos(2\varphi). \tag{2}$$

Here α' denotes the derivative of α w.r.t. x_1. Further, let α belong to the system of admissible functions

$$\mathcal{U}_{\rm ad} := \{\alpha \in C^{1,1}([0,1]);\ \hat{\alpha} \leqslant \alpha \leqslant \hat{\hat{\alpha}},\ |\alpha'| \leqslant L_1,\ |\alpha''| \leqslant L_2 \text{ a.e. in } (0,1)\}, \tag{3}$$

where $C^{1,1}$ denotes the space of functions whose first derivatives are Lipschitz continuous, $\hat{\alpha}$ and $\hat{\hat{\alpha}}$ are Lipschitz continuous functions and $0 < \alpha_{\min} \leqslant \hat{\alpha}$, implying that $b_\alpha \in (L^\infty(\Omega))^2$ and $\operatorname{div} b_\alpha, c_\alpha \in L^\infty(\Omega)$.

For a weak formulation we assume that there exists an extension of the Dirichlet boundary condition $\psi_D \in W^{1,2}(\Omega)$. This is obvious because ψ_D is constant on Γ_1. Further, we define the bilinear form a_α and the linear form f_α as follows:

$$a_\alpha(v,w) = \int_\Omega (\mathcal{A}\nabla v)\cdot\nabla w \,\mathrm{d}x + \int_\Omega (b_\alpha\cdot\nabla v + c_\alpha v)w\,\mathrm{d}x, \tag{4}$$

$$\langle f_\alpha, w\rangle = -a_\alpha(\psi_D, w), \tag{5}$$

and the space of test functions $V := \{v \in W^{1,2}(\Omega);\ \operatorname{Tr} v|_{\Gamma_1} = 0\}$, where Tr stands for the trace mapping. In what follows we denote by $\|\cdot\|_p$ and $\|\cdot\|_{k,p}$ the norm of $L^p(\Omega)$, and $W^{k,p}(\Omega)$, respectively.

Definition 1. The function $\psi \in W^{1,2}(\Omega)$ is said to be a weak solution of $(\mathrm{P}(\alpha))$ if $\psi_0 := \psi - \psi_D$ is an element of V and satisfies

$$a_\alpha(\psi_0, v) = \langle f_\alpha, v\rangle \quad \forall\, v \in V. \tag{6}$$

Lemma 1. *There exists a constant $C > 0$ independent of $\alpha \in \mathcal{U}_{\rm ad}$ such that*

$$|a_\alpha(v,w)| \leqslant C\|v\|_{1,2}\|w\|_{1,2}, \quad |\langle f_\alpha, w\rangle| \leqslant C\|w\|_{1,2} \tag{7}$$

hold for all $\alpha \in \mathcal{U}_{\rm ad}$ and all $v, w \in W^{1,2}(\Omega)$.

Lemma 2. *Let $\alpha \in \mathcal{U}_{\mathrm{ad}}$ and let any of the following conditions hold:*

(i) $c_\alpha - \frac{1}{2}\operatorname{div} b_\alpha \geqslant 0$ *a.e. in* Ω,

(ii) $\|c_\alpha - \frac{1}{2}\operatorname{div} b_\alpha\|_\infty C_F^2 < \gamma$, *where C_F is the constant from Friedrichs' inequality on V and γ is the smallest eigenvalue of $\mathcal{A}$.*

Then a_α is elliptic on V.

P r o o f. We rewrite the convective term using Green's formula:

$$\int_\Omega (b_\alpha \cdot \nabla v) v \,\mathrm{d}x = \int_{\partial\Omega} b_\alpha \cdot \nu \frac{v^2}{2} \,\mathrm{d}S - \int_\Omega \operatorname{div} b_\alpha \frac{v^2}{2} \,\mathrm{d}x \geqslant -\frac{1}{2} \int_\Omega \operatorname{div} b_\alpha v^2 \,\mathrm{d}x. \tag{8}$$

From this we see that

$$a_\alpha(v,v) \geqslant \gamma \|\nabla v\|_2^2 + \int_\Omega \Big(c_\alpha - \frac{1}{2}\operatorname{div} b_\alpha\Big) v^2 \,\mathrm{d}x \tag{9}$$

holds for every $v \in V$.

(i) In this case $a_\alpha(v,v) \geqslant \gamma\|\nabla v\|_2^2$ for all $v \in V$.

(ii) We estimate the last term from (9) using Hölder's and Friedrichs' inequalities, which yield

$$a_\alpha(v,v) \geqslant \Big(\gamma - \Big\|c_\alpha - \frac{1}{2}\operatorname{div} b_\alpha\Big\|_\infty C_F^2\Big) \|\nabla v\|_2^2. \tag{10}$$

□

Unfortunately, the assumption (i) of Lemma 2 can not be used in our case. A direct computation shows that

$$c_\alpha - \frac{1}{2}\operatorname{div} b_\alpha = \frac{\beta\alpha'}{2\alpha^2}(1 + 2\cos(2\varphi)), \tag{11}$$

as follows from (2), which cannot be positive for any $\alpha \in \mathcal{U}_{\mathrm{ad}}$. Therefore only (ii) will be used.

R e m a r k 1. Since Ω is a rectangle, it is easy to verify that Friedrichs' inequality on V holds with the constant $C_F := \operatorname{meas}\Omega = \pi$.

Theorem 3 (Existence and uniqueness)**.** *Let $\psi_D \in W^{1,2}(\Omega)$ and let*

$$\frac{3}{2}\pi^2 \frac{\beta L_1}{\alpha_{\min}^2} < \gamma. \tag{12}$$

Then for each $\alpha \in \mathcal{U}_{\mathrm{ad}}$ there exists a unique weak solution $\psi := \psi(\alpha)$ of $(\mathrm{P}(\alpha))$*. In addition,*

$$\|\psi\|_{1,2} \leqslant C\|\psi_D\|_{1,2}, \tag{13}$$

where $C > 0$ does not depend on α.

P r o o f. If (12) is satisfied, then the assumption (ii) of Lemma 2 holds, as follows from (11). Thus a_α is elliptic with a constant of ellipticity being independent of α. Existence and uniqueness of ψ satisfying (6) and (13) then follows from the Lax-Milgram lemma. □

The previous theorem assures solvability of (P(α)) only in the case of a dominating diffusion. At the end of this section we mention a more general existence (but not uniqueness) result based on Fredholm's theorem for linear compact mappings. Nevertheless it will not be used anywhere in this article.

Theorem 4. *Let $\alpha \in \mathcal{U}_{\rm ad}$ and $\psi_D \in W^{1,2}(\Omega)$. Then there exists at least one weak solution of* (P(α)) *if and only if*

$$\langle f_\alpha, x\rangle = 0 \tag{14}$$

for all $x \in V$ solving the homogeneous adjoint problem: $\forall\, y \in V$, $a_\alpha(y, x) = 0$.

We refer to [3] for further details concerning solvability of convection-diffusion problems.

3. Shape optimization problem

In what follows we will assume that the parameters of the model are chosen in such a way that (12) holds. Further we will denote by $\psi(\alpha)$ the weak solution of (P(α)). Let us define the cost function

$$J(\alpha) := \int_{\Gamma_2} |\psi(\alpha) - \psi_{\rm opt}|^2 \,\mathrm{d}S, \tag{15}$$

where $\psi_{\rm opt} \in L^2(\Gamma_2)$ is the desired distribution function on the outlet Γ_2. The shape optimization problem reads as follows:

$$\text{Find } \alpha^* \in \mathcal{U}_{\rm ad} \text{ such that } J(\alpha^*) = \min_{\alpha\in\mathcal{U}_{\rm ad}} J(\alpha). \tag{$\mathbb{P}$}$$

Let us remark that in fact ($\mathbb{P}$) is an optimal control problem since $\psi(\alpha)$ is computed on the fixed domain Ω and the control α appears only in the coefficients of the state equation.

3.1. Existence of optimal shape

We will show that ($\mathbb{P}$) has a solution using the classical Bolzano-Weierstrass theorem for continuous functions on compact sets.

Definition 2. We define the convergence in $\mathcal{U}_{\rm ad}$ as follows:

$$\alpha_n \rightsquigarrow \alpha \overset{\rm def}{\Leftrightarrow} \alpha_n \rightrightarrows \alpha \ \text{ in } \ [0,1] \quad \text{and} \quad \alpha_n' \rightrightarrows \alpha' \ \text{ in } \ [0,1]. \tag{16}$$

From the well known Arzelà-Ascoli theorem it follows that $\mathcal{U}_{\rm ad}$ is compact with respect to above defined convergence.

Lemma 5. *Let $\alpha_n \rightsquigarrow \alpha$ in $\mathcal{U}_{\rm ad}$. Then*

$$\psi(\alpha_n) \to \psi(\alpha) \quad \textit{strongly in } \ W^{1,2}(\Omega). \tag{17}$$

P r o o f. It is easy to see that $b_{\alpha_n} \rightrightarrows b_\alpha$ and $c_{\alpha_n} \rightrightarrows c_\alpha$ in $\overline{\Omega}$. From Theorem 3 it follows that the solutions $\psi_n := \psi(\alpha_n)$ of $(\mathrm{P}(\alpha_n))$ are bounded:

$$\|\psi_n\|_{1,2} \leqslant C\|\psi_D\|_{1,2}, \tag{18}$$

where C is independent of α_n. Therefore a subsequence $\{\psi_{n_k}\}$ exists and converges weakly to some ψ in $W^{1,2}(\Omega)$. Moreover $\psi - \psi_D \in V$, $a_{n_k}(\psi_{n_k}, \varphi) \to a_\alpha(\psi, \varphi)$ for all $\varphi \in V$, i.e. $\psi = \psi(\alpha)$ is the solution of $(\mathrm{P}(\alpha))$. Since this solution is unique, the whole sequence $\{\psi_n\}$ tends weakly to $\psi(\alpha)$. Finally we use the ellipticity of a_n and Rellich's theorem to obtain strong convergence:

$$\begin{aligned} C\|\psi_n - \psi(\alpha)\|_{1,2}^2 &\leqslant a_n(\psi_n - \psi(\alpha), \psi_n - \psi(\alpha)) = \underbrace{a_n(\psi_n, \psi_n - \psi(\alpha))}_{=0} \\ &- \int_\Omega (\mathcal{A}\nabla\psi(\alpha)) \cdot \underbrace{\nabla(\psi_n - \psi(\alpha))}_{\rightharpoonup 0 \text{ in } L^2(\Omega)} + \underbrace{(b_n \cdot \nabla\psi(\alpha) + c_n\psi(\alpha)}_{\text{bounded in } L^2(\Omega)} \underbrace{(\psi_n - \psi(\alpha))}_{\to 0 \text{ in } L^2(\Omega)} \, \mathrm{d}x. \end{aligned} \tag{19}$$

$\square$

Lemma 6. *J is continuous on $\mathcal{U}_{\rm ad}$.*

P r o o f. Let $\alpha_n \rightrightarrows \alpha$ in $[0,1]$. From Lemma 5 it follows that $\psi(\alpha_n) \to \psi(\alpha)$ in $W^{1,2}(\Omega)$. The continuous imbedding of $W^{1,2}(\Omega)$ into $L^2(\Gamma_2)$ yields

$$\operatorname{Tr}\psi(\alpha_n)|_{\Gamma_2} \to \operatorname{Tr}\psi(\alpha)|_{\Gamma_2} \quad \text{in } \ L^2(\Gamma_2) \tag{20}$$

and consequently $J(\alpha_n) \to J(\alpha)$. $\square$

Theorem 7 (Existence). *Problem* ($\mathbb{P}$) *has a solution.*

Proof. Since J is continuous and $\mathcal{U}_{\rm ad}$ is compact, the Bolzano-Weierstrass theorem says that J attains its minimum on $\mathcal{U}_{\rm ad}$. $\square$

3.2. Sensitivity analysis

We have proved that the mappings $\alpha \mapsto \psi(\alpha)$ and $\alpha \mapsto J(\alpha)$ are continuous on $\mathcal{U}_{\rm ad}$. In this subsection their differentiability will be studied using the Implicit Function Theorem and the adjoint equation technique. Finally we derive the optimality condition for ($\mathbb{P}$).

Lemma 8. *The mapping $\alpha \mapsto \psi(\alpha)$ is continuously (Fréchet) differentiable on $\mathcal{U}_{\rm ad}$.*

Proof. Let us define the function $F\colon \mathcal{U}_{\rm ad} \times V \to V^*$ by

$$F(\alpha,\psi) := A_\alpha(\psi) - f_\alpha = A_\alpha(\psi + \psi_D), \tag{21}$$

where $A_\alpha \in \mathcal{L}(W^{1,2}(\Omega), V^*)$, $\langle A_\alpha(\psi), \varphi\rangle = a_\alpha(\psi,\varphi)\ \forall\, \psi \in W^{1,2}(\Omega)$, $\varphi \in V$. Then $F(\alpha, \psi(\alpha) - \psi_D) = 0$ for all $\alpha \in \mathcal{U}_{\rm ad}$ and the Implicit Function Theorem yields

$$\psi'(\alpha)h = -A_\alpha^{-1}\Big(\frac{\partial A_\alpha}{\partial \alpha}(\psi(\alpha))h\Big) \quad \text{for any } \ h \in C^{1,1}([0,1]). \tag{22}$$

Indeed, A_α is a bounded linear mapping of $W^{1,2}(\Omega)$ onto V^*, thus A_α^{-1} is bounded, too. Since b_α and c_α are continuously differentiable with respect to α, so is A_α and

$$\Big\langle \frac{\partial A_\alpha}{\partial \alpha}(\psi)h, \varphi \Big\rangle = \int_\Omega \Big(\frac{\partial b_\alpha}{\partial \alpha} h \cdot \nabla\psi + \frac{\partial c_\alpha}{\partial \alpha} h\psi\Big)\varphi \,\mathrm{d}x \tag{23}$$

for $h \in C^{1,1}([0,1])$. $\square$

We are interested in differentiability of the cost function J. In order to express J', let us denote $\mathcal{J}(\psi) := \int_{\Gamma_2} |\psi - \psi_{\rm opt}|^2 \,\mathrm{d}S$ and introduce the adjoint state $p \in V$:

$$\langle A_\alpha(\varphi), p\rangle = 2\int_{\Gamma_2} (\psi(\alpha) - \psi_{\rm opt})\varphi \,\mathrm{d}S \quad \text{for all } \ \varphi \in V. \tag{24}$$

Note that (24) is uniquely solvable since a_α is elliptic and the right-hand side is a bounded linear functional on V.

Lemma 9. *J is continuously (Fréchet) differentiable on $\mathcal{U}_{\mathrm{ad}}$ and*

$$J'(\alpha)h = -\Big\langle \frac{\partial A_\alpha}{\partial \alpha}(\psi(\alpha))h, p\Big\rangle, \quad h \in C^{1,1}([0,1]), \tag{25}$$

where p is a solution of (24).

Proof. Since J does not depend explicitly on α, its derivative is

$$J'(\alpha)h = \mathcal{J}'(\psi(\alpha))\psi'(\alpha)h = \langle A_\alpha(\psi'(\alpha)h), p\rangle = -\Big\langle \frac{\partial A_\alpha}{\partial \alpha}(\psi(\alpha))h, p\Big\rangle, \tag{26}$$

as follows from (24) and (22). Continuity of J' on $\mathcal{U}_{\mathrm{ad}}$ follows from Lemma 8. □

Theorem 10 (Optimality condition). *Let $\alpha^* \in \mathcal{U}_{\mathrm{ad}}$ be a solution of* ($\mathbb{P}$). *Then*

$$\int_\Omega \Big(\frac{\partial b_{\alpha^*}}{\partial \alpha}(\tilde\alpha - \alpha^*)\cdot \nabla\psi(\alpha^*) + \frac{\partial c_{\alpha^*}}{\partial \alpha}(\tilde\alpha - \alpha^*)\psi(\alpha^*)\Big) p \, \mathrm{d}x \leqslant 0 \tag{27}$$

holds for all $\tilde\alpha \in \mathcal{U}_{\mathrm{ad}}$, where p is a solution of (24) *with $\alpha := \alpha^*$.*

4. Approximation and numerical solution

We shall solve numerically an approximate optimization problem. Therefore we discretize the state problem and the set of admissible functions.

Let $\mathcal{U}^n_{\mathrm{ad}}$ be a set of Bézier functions of the order $n+1$ such that $\mathcal{U}^n_{\mathrm{ad}} \subset \mathcal{U}_{\mathrm{ad}}$. With each element of $\mathcal{U}^n_{\mathrm{ad}}$ of the form

$$\alpha_n(x_1) := \sum_{i=0}^{n+1} a_i \binom{n+1}{i} x_1^i (1-x_1)^{n+1-i}$$

we associate the vector $a := (a_1, \ldots, a_n)^{\mathrm{T}} \in U^n$. (Since the ends of the curves α_n are fixed, a_0 and a_{n+1} are also fixed). Here U^n is chosen so that $a \in U^n \Leftrightarrow \alpha_n \in \mathcal{U}^n_{\mathrm{ad}}$.

4.1. State problem

The state problem (6) with fixed α is solved using the Finite Element Method (FEM). Let $\mathcal{T}_h$ denote a partition of Ω into triangles. We define the finite dimensional subspace of V:

$$V_h := \{v_h \in V\,;\ v_h|_T \in P_1(T)\ \forall\, T \in \mathcal{T}_h\}. \tag{28}$$

Instead of the standard Galerkin FEM approximation we use a stabilized variant, namely the streamline upwind Petrov-Galerkin (SUPG) method. The discrete state problem is then defined as the following:

$$
(\mathrm{P}_h(\alpha)) \qquad \begin{cases} \text{Find } \psi_h := \psi_h(\alpha) \in W^{1,2}(\Omega) \text{ such that } \psi_h - \psi_D \in V_h \text{ and} \\ a_\alpha(\psi_h, v_h) + \sum_{T \in \mathcal{T}_h} \int_T \tau_T (b_\alpha \cdot \nabla \psi_h + c_\alpha \psi_h) b_\alpha \cdot \nabla v_h \,\mathrm{d}x = 0 \ \forall\, v_h \in V_h. \end{cases}
$$

Here τ_T is a positive upwind parameter depending on the local Peclet number.

Let $\{\omega_i\}_{i=1}^N$ be the Lagrangean basis of V_h. Then $\psi_h = \sum_{i=1}^N q_i \omega_i$, where $q := q(a) := (q_1, \ldots, q_N)^{\mathrm{T}}$ contains the nodal values of ψ_h. Using this notation, $(\mathrm{P}_h(\alpha))$ can be rewritten as the system of linear algebraic equations

$$
R(a, q(a)) = 0, \tag{29}
$$

which is assembled elementwise in the following way:

$$
R(a, q) = \sum_{T \in \mathcal{T}_h} R_T(a, q), \tag{30}
$$

$$
(R_T)_i(a, q) = \int_T (\mathcal{A} \nabla \psi_h) \cdot \nabla \omega_i + (b_{\alpha_n} \cdot \nabla \psi_h + c_{\alpha_n} \psi_h) \tilde{\omega}_i \,\mathrm{d}x, \tag{31}
$$

$$
\tilde{\omega}_i := \omega_i + \tau_T b_{\alpha_n} \cdot \nabla \omega_i. \tag{32}
$$

The sparse linear system (29), with $a \in U^n$ fixed, is solved with help of the package SuperLU (see [2] for documentation).

4.2. Optimization problem

The algebraic form of the cost function reads as

$$
\mathcal{J}_h(q) := \int_{\Gamma_2} \left(\sum_{i=1}^N q_i \omega_i - \psi_{\mathrm{opt}} \right)^2 \mathrm{d}S. \tag{33}
$$

We solve numerically the following mathematical programming problem:

$$
(\mathbb{P}_h) \qquad \text{Find } a^* \in U^n \text{ such that } \mathcal{J}_h(q(a^*)) = \min_{a \in U^n} \mathcal{J}_h(q(a)),
$$

where $q(a)$ is the solution of (29) with a given a. Since U^n is compact and $\mathcal{J}_h$ is clearly continuous, $\mathbb{P}_h$ has a solution.

For the numerical minimization we use the package KNITRO which uses trust region method based on interior point techniques (see [1] for algorithm description).

The minimization method requires the evaluation of $\nabla \mathcal{J}_h(q(a))$ at a given point a. The exact partial derivatives of $\mathcal{J}_h$ are computed using the adjoint equation technique:

$$\frac{\partial \mathcal{J}_h(q(a))}{\partial a_k} = -p^{\mathrm{T}}\Big(\frac{\partial R(a,q(a))}{\partial a_k}\Big), \quad k = 1,\dots,n, \tag{34}$$

where $p := p(a)$ is the solution of the adjoint equation

$$\Big(\frac{\partial R(a,q(a))}{\partial q}\Big)^{\mathrm{T}} p = \frac{\partial \mathcal{J}_h(q(a))}{\partial q}. \tag{35}$$

Note that equations (34), (35) remain valid for nonlinear state problems, too. As the hand-coding of the partial derivatives appearing in (34) and (35) is time consuming and error-prone, we compute them with the aid of automatic differentiation.

4.3. Automatic differentiation

Automatic differentiation (AD) technique is based on the chain rule of differentiation, and it exploits the fact that every computer program (including our finite element code) executes a sequence of elementary arithmetic operations (see e.g. [4], [7] for details).

The automatic differentiation works as follows. A set of independent variables $w_1,\dots,w_M$ is defined in the beginning of the computation. In this case, the independent variables are the nodal values of the FEM solution $q_1,\dots,q_N$ and the design parameters $a_1,\dots,a_n$.

Consider now an elementary function $\Phi(y_1,\dots y_m)$ whose arguments depend on (some of) the independent variables: $y_i = y_i(w_1,\dots w_M)$. For our finite element code it was sufficient to implement only the basic elementary functions like $+$, $-$, $*$ and $/$, for which it holds that $m \leqslant 2$. Chain rule of differentiation applied to the assignment $z = \Phi(y_1,\dots y_m)$ gives

$$\frac{\partial z}{\partial w_j} = \sum_{k=1}^{m} \frac{\partial \Phi}{\partial y_k}\frac{\partial y_k}{\partial w_j}. \tag{36}$$

The partial derivatives $\partial\Phi/\partial y_k$ of these functions are readily obtained, and thus the partial derivatives $\partial z/\partial w_j$ can be computed as long as the partial derivatives $\partial y_k/\partial w_j$ are known.

Our implementation of the AD is as follows. We define a composite data type `CVar`, which holds the value of a real variable and its partial derivatives with respect to the independent variables $w_1,\dots,w_M$. We can now represent the variables $y_1,\dots,y_m, z$

with this data type, and implement the function Φ such that it computes both the result z and its partial derivatives.

A unique global identification number is assigned to each independent variable. In the following we assume that the identification number of w_i is i. The object of type `CVar` representing a generic real variable x includes a vector of integers V_{ind} and a vector of real numbers d. The vector V_{ind} holds the set $n_z(x) = \{i\colon \partial x/\partial w_i \neq 0\}$ in increasing order, and d holds the values $d(j) = \partial x/\partial w_{V_{\text{ind}}(j)}$.

We initialize the partial derivatives $\partial w_i/\partial w_i = 1$ for the objects representing the independent variables, and apply the automatic differentiation procedure at every step while assembling the residual and performing the cost functional evaluation. Eventually, the objects representing the residual components and the cost functional value include all the necessary partial derivatives.

Possible source of inefficiency lies in the fact that typically M is large, so that many partial derivatives might have to be computed. But in FEM, each residual component depends only on few degrees of freedom. The same holds also for all the intermediate variables generated in the execution chain of the residual assembly. We notice that $j \notin n_z(y_i)$ for all $i \in 1\dots m \implies \partial z/\partial w_j = 0$. Therefore, we only need to go through those indices that belong to $n_z(y_i)$ for some i. The fact that the array V_{ind} is ordered enables us to build an implementation where we only have to go through the vectors V_{ind} and d of each y_i once during the computation of ∇z. The total computational complexity of the gradient evaluation is thus $\mathcal{O}\Big(\sum_{i=1}^{m} \#n_z(y_i)\Big)$.

We used the operator overloading property of C++ to "hide" the implementation of the AD from the user. The elementary operators were overloaded so that the user can simply write for example `z = y1 + y2`, where `z`, `y1` and `y2` are of type `CVar`, and the compiler takes care of calling the appropriate function implementing the automatic differentiation.

4.4. Numerical examples

In the following numerical example the matrix $\mathcal{A}$ is of the form $\begin{pmatrix} D_T & 0 \\ 0 & D_R \end{pmatrix}$, where D_T is the translational dispersion coefficient and D_R the rotational dispersion coefficient. We made two computations with $D_T = 10^{-5}$ and with different values of D_R. The velocity coefficient β is set to 0.1. Due to symmetry of the coefficients and boundary conditions, the state problem is solved only in the subdomain $(0,1) \times (0, \frac{1}{2}\pi)$. The finite element mesh is structured and consists of 2552 linear triangle elements. In the vicinity of the point $[1,0]$ the mesh is refined due to high gradient of the solution. The function α characterizing the height of the contraction is discretized using Bézier function with 30 control points. The parameters defining the set $\mathcal{U}_{\text{ad}}$

are:

$$\hat{\alpha}(x_1) = 0.1 - 0.33x_1 + 0.345x_1^2 - 0.105x_1^3,$$
$$\hat{\hat{\alpha}}(x_1) = 0.1(1 - x_1) + 0.01x_1,$$
$$L_1 = 10, \quad L_2 = 100.$$

The target distribution is $\psi_{\text{opt}}(\varphi) = \pi^{-1}$. We started the computation with the initial guess equal to traditional linearly tapered design ($\hat{\hat{\alpha}}$).

In the first computation the rotational dispersion coefficient was set to $D_R = 5$. After 107 iterations the value of the cost function decreased from 5.379×10^{-1} to 1.918×10^{-3} as the optimality error (specified in the user's manual of KNITRO) reached 10^{-5}. The initial and final geometry of the contraction is shown on Fig. 2, the initial and final orientation distributions at the outlet are shown on Fig. 3. Contour plots of the initial and final orientation distribution in the computational domain are shown on Fig. 4.

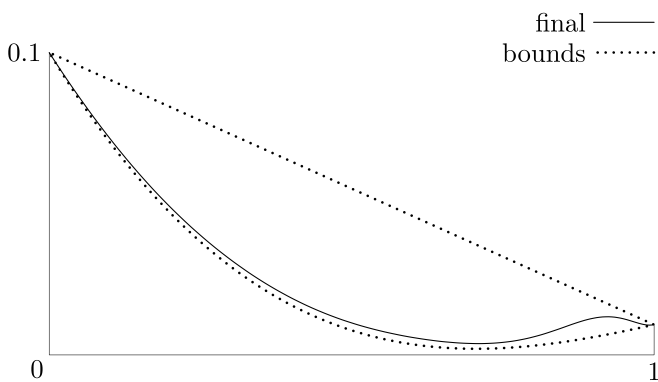

Figure 2. The final geometry of the contraction.

In the second computation we set $D_R = 0.05$. After 9 iterations the value of the cost function decreased from 7.452 to 6.315×10^{-1} as the optimality error reached 10^{-6}. The initial and final geometry of the contraction is shown on Fig. 5, the initial and final orientation distributions at the outlet are shown on Fig. 6. Contour plots of the initial and final orientation distribution in the computational domain are shown on Fig. 7.

There is no reason to assume that the cost function is convex, therefore the found minima are possibly only local. However our first result is very similar to the one from [11], where the authors used different methods and initial guesses. Thus, there is a chance that the final design is close to the global minimum.

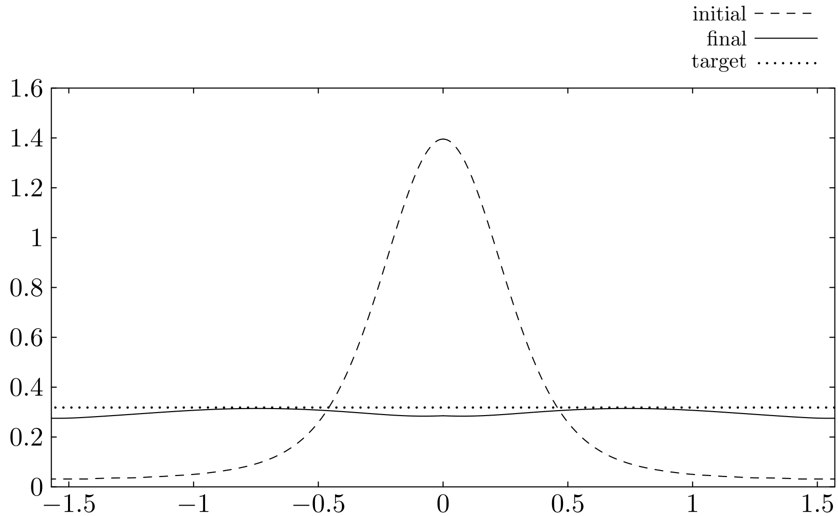

Figure 3. The initial and final orientation distribution at the outlet.

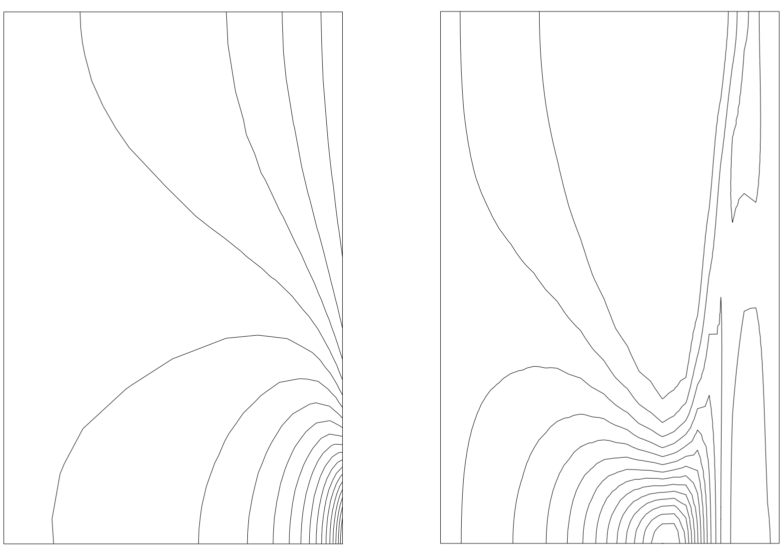
Figure 4. Contour plots of the initial and final solution ψ_h (in the computational domain $(0,1) \times (0, \frac{1}{2}\pi)$).

It is easy to verify that the parameters used in these numerical examples do not satisfy (12). However the computational problem does not seem to be ill posed—the resulting stiffness matrix is always regular also without using upwind. The obtained solution of $(\mathrm{P}_h(\alpha))$ is independent of the mesh structure, provided that the mesh is fine enough. Then there are several questions arising: Is the continuous

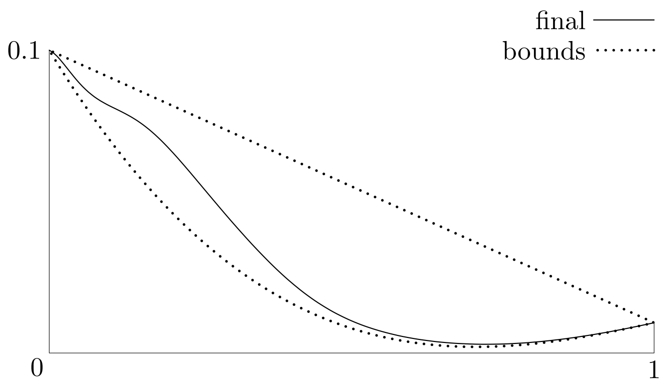

Figure 5. The final geometry of the contraction.

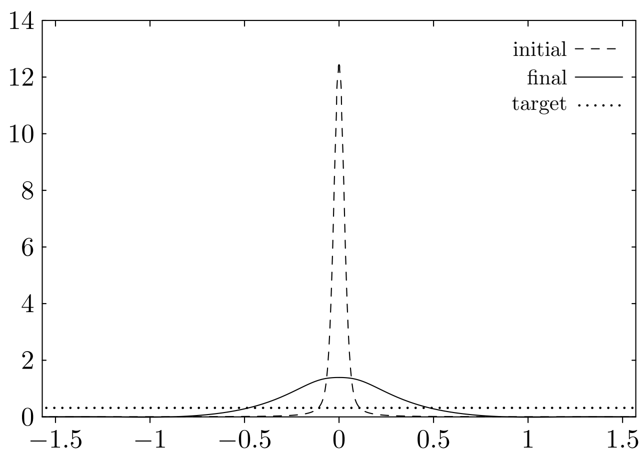

Figure 6. The initial and final orientation distribution at the outlet.

problem (P(α)) still uniquely solvable if (12) is not satisfied? If not, is it solvable? Are the solutions of (P$_h$(α)) bounded as $h \to 0+$? These questions will be studied in future projects. Replacing the simple one-dimensional flow by a more realistic model will be also considered.

References

[1] *R. Byrd, J. C. Gilbert, and J. Nocedal*: A trust region method based on interior point techniques for nonlinear programming. Math. Program. A *89* (2000), 149–185. zbl

[2] *J. W. Demmel, S. C. Eisenstat, J. R. Gilbert, X. S. Li, and J. W. H. Liu*: A supernodal approach to sparse partial pivoting. SIAM J. Matrix Anal. Appl. *20* (1999), 720–755. zbl

[3] *D. Gilbarg, N. S. Trudinger*: Elliptic Partial Differential Equations of Second Order. Springer-Verlag, Berlin, 2001. zbl

[4] *A. Griewank*: Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation. SIAM, Philadelphia, 2000. zbl

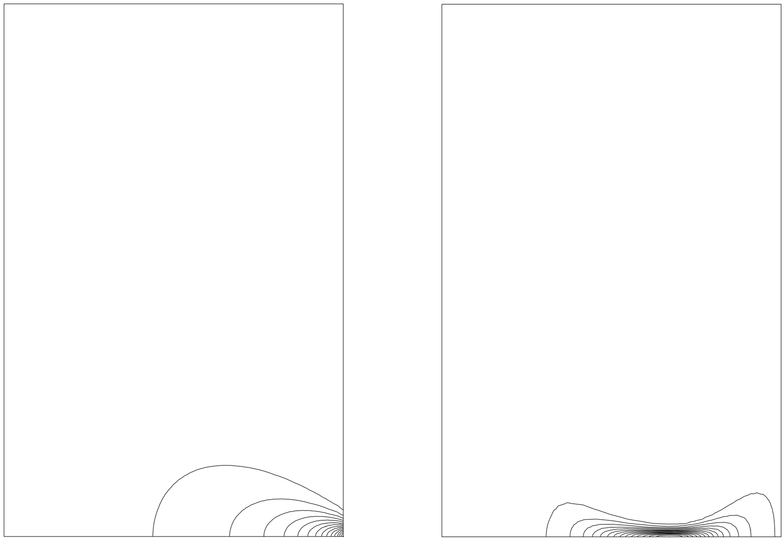

Figure 7. Contour plots of the initial and final solution ψ_h (in the computational domain $(0,1)\times(0,\frac{1}{2}\pi)$).

[5] *J. Hämäläinen*: Mathematical Modelling and Simulation of Fluid Flows in Headbox of Paper Machines. University of Jyväskylä, Jyväskyä, 1993. zbl

[6] *J. Hämäläinen, R. A. E. Mäkinen, and P. Tarvainen*: Optimal design of paper machine headboxes. Int. J. Numer. Methods Fluids *34* (2000), 685–700. zbl

[7] *J. Haslinger, R. A. E. Mäkinen*: Introduction to Shape Optimization: Theory, Approximation, and Computation. SIAM, Philadelphia, 2003. zbl

[8] *J. Haslinger, J. Málek, and J. Stebel*: Shape optimization in problems governed by generalised Navier-Stokes Equations: Existence analysis. Control Cybern. *34* (2005), 283–303.

[9] *M. Křížek, P. Neittaanmäki*: Finite Element Approximation of Variational Problems and Applications. Longman Academic, Scientific & Technical, Harlow, 1990. zbl

[10] *O. A. Ladyzhenskaya, N. N. Ural'tseva*: Linear and Quasilinear Elliptic Equations. Academic Press, New York-London, 1968. zbl

[11] *R. A. E. Mäkinen, J. Hämäläinen*: Optimal control of a turbulent fibre suspension flowing in a planar contraction. Commun. Numer. Meth. Eng.; Published Online: 13 Dec 2005, DOI: 10.1002/cnm.833.

[12] *A. Olson, I. Frigaard, C. Chan, and J. P. Hämäläinen*: Modelling a turbulent fibre suspension flowing in a planar contraction: The one-dimensional headbox. Int. J. Multiphase Flow *30* (2004), 51–66.

Authors' addresses: *J. Stebel*, Department of Numerical Mathematics, Faculty of Mathematics and Physics, Charles University in Prague, Sokolovská 83, 186 75 Praha 8, Czech Republic, e-mail: `stebel@karlin.mff.cuni.cz`; *R. A. E. Mäkinen*, Department of Mathematical Information Technology, University of Jyväskylä, PO Box 35 (Agora), FI-40014 Jyväskylä, Finland, e-mail: `rainom@it.jyu.fi`; *J. I. Toivanen*, Department of Mathematical Information Technology, University of Jyväskylä, PO Box 35 (Agora), FI-40014 Jyväskylä, Finland, e-mail: `jitoivan@cc.jyu.fi`.