Hamburger Beiträge
zur Angewandten Mathematik

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Nr. 2008-09
August 2008

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Nov. 26, 2008

Abstract We investigate a semi-smooth Newton method for the numerical solution of optimal control problems subject to differential-algebraic equations (DAEs) and mixed control-state constraints. The necessary conditions are stated in terms of a local minimum principle. By use of the Fischer-Burmeister function the local minimum principle is transformed into an equivalent nonlinear and semi-smooth equation in appropriate Banach spaces. This nonlinear and semi-smooth equation is solved by a semi-smooth Newton method. We extend known local and global convergence results for ODE optimal control problems to the DAE optimal control problems under consideration. Special emphasis is layed on the calculation of Newton steps which are given by a linear DAE boundary value problem. Regularity conditions which ensure the existence of solutions are provided. A regularization strategy for inconsistent boundary value problems is suggested. Numerical illustrations for the optimal control of a pendulum and for the optimal control of discretized Navier-Stokes equation conclude the article.

Keywords Optimal control · Semi-smooth Newton method · Differential-algebraic equations · Control-state constraints · Global convergence

Mathematics Subject Classification (2000) 49J15 · 49J52 · 49M15

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1 Introduction

Differential-algebraic equations (DAEs) are composite systems of differential equations and algebraic equations and often are viewed as differential equations on manifolds. In its most general form a DAE is an implicit ordinary differential equation (ODE) of type

$$G(\xi(t), \xi'(t), u(t)) = 0. \tag{1}$$

If the partial derivative $G'_{\xi'}$ happens to be non-singular, then (1) is just an ODE in implicit form and the implicit function theorem allows to solve (1) for ξ' in order to obtain an explicit ODE. The more interesting case occurs if the partial derivative $G'_{\xi'}$ is singular. In this case (1) cannot be solved directly for ξ' and (1) includes differential equations and algebraic equations at the same time. Theoretical properties and numerical methods for solving equations of such type are discussed intensively since the early 1970ies, see Brenan et al. [2], Hairer and Wanner [15], and Kunkel and Mehrmann [20]. Although DAEs seem to be very similar to ODEs they possess different solution properties, see Petzold [23]. Particularly, DAEs possess different stability properties compared to ODEs and initial values have to be defined properly to guarantee at least locally unique solutions. At present, (1) is too general and therefore too challenging to being tackled theoretically or numerically. In this article we restrict the discussion to semi-explicit DAEs of type

$$x'(t) = f(x(t), y(t), u(t)), \tag{2}$$

$$0 = g(x(t)), \tag{3}$$

where the state ξ in (1) is decomposed into components x and y. Herein, $x(\cdot)$ is referred to as differential variable and $y(\cdot)$ is called algebraic variable. Correspondingly, (2) is called differential equation and (3) algebraic equation. The control variable u is an external input which allows to control the DAE in an appropriate way.

The most important application that fits into (2)-(3) are mechanical multibody systems with Gear-Gupta-Leimkuhler stabilization, see [8]. The latter have the following structure

$$\begin{aligned}
x' &= v - g'(x)^\top \mu, \\
v' &= M(x)^{-1} \left(f(x, v, u) - g'(x)^\top \lambda \right), \\
0 &= g(x), \\
0 &= g'(x)v.
\end{aligned}$$

Moreover, problems in process engineering, electrical engineering, and, as we shall see later, discretized Navier-Stokes equations lead to DAEs of type (2)-(3). Often, the control u has to be chosen such that a given performance index is minimized subject to constraints. This leads to the following optimal control problem subject to mixed control-state constraints (OCP):

$$\begin{array}{ll} \text{Minimize} & \displaystyle\int_0^1 f_0(x(t), y(t), u(t))dt \\ \text{w.r.t.} & x \in W^{1,\infty}([0,1], \mathbb{R}^{n_x}), y \in L^\infty([0,1], \mathbb{R}^{n_y}), u \in L^\infty([0,1], \mathbb{R}^{n_u}), \\ \text{s.t.} & \text{DAE } (2) - (3), \\ & \psi(x(0), x(1)) = 0, \\ & c(x(t), y(t), u(t)) \leq 0 \text{ a.e. in } [0,1]. \end{array}$$

Without loss of generality the discussion is restricted to autonomous problems on the fixed time interval $[0,1]$. The functions $f_0 : \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_u} \to \mathbb{R}$, $f : \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_u} \to \mathbb{R}^{n_x}$, $g : \mathbb{R}^{n_x} \to \mathbb{R}^{n_y}$, $\psi : \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \to \mathbb{R}^{n_\psi}$, $c : \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_u} \to \mathbb{R}^{n_c}$ are supposed to be at least twice continuously differentiable w.r.t. to all arguments. As usual, the Banach space $L^\infty([0,1], \mathbb{R}^n)$ consists of all measurable functions $h : [0,1] \to \mathbb{R}^n$ with

$$\|h\|_\infty := \operatorname*{ess\,sup}_{0 \leq t \leq 1} \|h(t)\| < \infty,$$

where $\|\cdot\|$ denotes the Euclidian norm on $\mathbb{R}^n$. For $1 \leq r < \infty$ the Banach spaces $L^r([0,1], \mathbb{R}^n)$ consist of all measurable functions $h : [0,1] \to \mathbb{R}^n$ with

$$\|h\|_r := \left(\int_0^1 \|h(t)\|^r \, dt \right)^{1/r} < \infty.$$

For $1 \leq r \leq \infty$ the Banach spaces $W^{1,r}([0,1], \mathbb{R}^n)$ consist of all absolutely continuous functions $h : [0,1] \to \mathbb{R}^n$ with

$$\|h\|_{1,r} := \max\{\|h\|_r, \|h'\|_r\} < \infty.$$

Most numerical approaches for OCP and more general DAE optimal control problems, respectively, are based on direct discretization in combination with shooting techniques, compare Pantelides et al. [22], Gritsis et al. [14], Schulz et al. [29], and Gerdts [11]. These methods proved their capability in various practical applications. Nevertheless, the computational effort grows at a nonlinear rate with the number of grid points used for discretization.

Alternative method try to satisfy first-order necessary optimality conditions. Optimality conditions for OCP can be found in Gerdts [9]. Further results for more general DAEs were derived by Roubicek and Valásek [26] and Backes [1]. However, the exploitation of the necessary conditions leads to a nonlinear multi-point boundary value problem which has to be solved numerically. Especially in the presence of control-state constraints this requires a sufficiently good initial guess of the solution, the Lagrange multipliers and the sequence of active and in-active constraints. For demanding problems obtaining a good initial guess is crucial. Often, direct methods can be used to provide an initial guess.

Our intention is to analyze the local and global convergence properties of an alternative method – the semi-smooth Newton's method. The method is based on a reformulation of the necessary optimality conditions and it was analyzed for optimal control problems subject to ODEs in Gerdts [13]. A brief outline of the essential ideas of the algorithm is as follows. The reformulation of the necessary conditions leads to the semi-smooth equation

$$F(z) = 0, \qquad F : Z \to Y,$$

where Z and Y are appropriate Banach spaces. Application of the globalized semi-smooth Newton's method generates sequences $\{z^k\}$, $\{d^k\}$ and $\{\alpha_k\}$ related by the iteration

$$z^{k+1} = z^k + \alpha_k d^k, \qquad k = 0, 1, 2, \ldots.$$

Herein, the search direction d^k is the solution of the linear operator equation $V_k(d^k) = -F(z^k)$ and the step length $\alpha_k > 0$ is determined by a line-search procedure of Armijo's type for a suitably defined merit function. The linear operator V_k is chosen from an appropriately defined generalized Jacobian $\partial_* F(z^k)$.

The semi-smooth Newton's method was investigated in finite dimensions amongst others by Qi [24] and Qi and Sun [25]. Extensions to infinite spaces can be found in Kummer [18,19], Chen et al. [4], Ulbrich [30,31], and Gerdts [13].

The paper is organized as follows. Section 2 introduces the semi-smooth Newton's method for OCP and establishes the locally superlinear convergence using results in Gerdts [13]. In Section 3 details of the computation of the search direction are shown. It turns out that the search direction solves a linear DAE boundary value problem. Sufficient conditions for the existence of the Newton direction are provided. Section 4 discusses global convergence properties of the semi-smooth Newton's method. Finally, numerical illustrations are presented in Section 5.

2 Local Convergence of the Semi-Smooth Newton's Method

The (augmented) Hamilton function $H : \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_c} \to \mathbb{R}$ is defined by

$$H(x, y, u, \lambda_f, \lambda_g, \eta) := \\ f_0(x, y, u) + \lambda_f^\top f(x, y, u) + \lambda_g^\top g'_x(x) f(x, y, u) + \eta^\top c(x, y, u).$$

We summarize the minimum principle for OCP, cf. Gerdts [10,9]. Let (x_*, y_*, u_*) be a (weak) local minimum of OCP and

(i) let φ, f_0, f, ψ, c be continuous w.r.t. all arguments and continuously differentiable w.r.t. x, y, and u. Let g be twice continuously differentiable w.r.t. all arguments.

(ii) let the matrix $M := g'_x \cdot f'_y$ be non-singular a.e. in $[0,1]$ and let M^{-1} be essentially bounded in $[0,1]$. Furthermore, let

$$\hat{M} := g'_x \cdot \left(f'_y - f'_u (c'_u)^+ c'_y\right)$$

be non-singular with essentially bounded inverse $\hat{M}^{-1}$ a.e. in $[0,1]$. Herein, $(c'_u)^+ = c'^{\top}_u \left(c'_u c'^{\top}_u\right)^{-1}$ denotes the pseudo-inverse of c'_u.

(iii) let

$$\operatorname{rank}\left(c'_u(x_*(t), y_*(t), u_*(t))\right) = n_c$$

hold a.e. in $[0,1]$, and let the Mangasarian-Fromowitz constraint qualification hold, cf. Gerdts [9].

Then there exist multipliers $\zeta_* \in \mathbb{R}^{n_y}$, $\sigma_* \in \mathbb{R}^{n_\psi}$, $\lambda_{f,*} \in W^{1,\infty}([0,1], \mathbb{R}^{n_x})$, $\lambda_{g,*} \in L^\infty([0,1], \mathbb{R}^{n_y})$, and $\eta_* \in L^\infty([0,1], \mathbb{R}^{n_c})$ with

$$x'_*(t) - f(x_*(t), y_*(t), u_*(t)) = 0, \tag{4}$$

$$g(x_*(t)) = 0, \tag{5}$$

$$\lambda'_{f,*}(t) + H'_x(x_*(t), y_*(t), u_*(t), \lambda_{f,*}(t), \lambda_{g,*}(t), \eta_*(t))^\top = 0, \tag{6}$$

$$H'_y(x_*(t), y_*(t), u_*(t), \lambda_{f,*}(t), \lambda_{g,*}(t), \eta_*(t))^\top = 0, \tag{7}$$

$$\psi(x_*(0), x_*(1)) = 0, \tag{8}$$

$$\lambda_{f,*}(0) + \psi'_{x_0}(x_*(0), x_*(1))^\top \sigma_* + g'_x(x_*(0))^\top \zeta_* = 0, \tag{9}$$

$$\lambda_{f,*}(1) - \psi'_{x_1}(x_*(0), x_*(1))^\top \sigma_* = 0, \tag{10}$$

$$H'_u(x_*(t), y_*(t), u_*(t), \lambda_{f,*}(t), \lambda_{g,*}(t), \eta_*(t))^\top = 0. \tag{11}$$

Furthermore, the complementarity conditions hold a.e. in $[0,1]$:

$$\eta_*(t) \geq 0, \qquad c(x_*(t), y_*(t), u_*(t)) \leq 0, \qquad \eta_*(t)^\top c(x_*(t), y_*(t), u_*(t)) = 0. \tag{12}$$

Unfortunately, these necessary conditions are not directly solvable for $z_* := (x_*, y_*, u_*, \lambda_{f,*}, \lambda_{g,*}, \eta_*, \zeta_*, \sigma_*)$ owing to the complementarity conditions. Therefore, the subsequent considerations aim at the reformulation of this set of equalities and inequalities as an equivalent system of equations, which will be solved by a generalized version of Newton's method. Throughout the rest of the paper for brevity we will use the notation $f[t]$ for $f(x(t), y(t), u(t))$ and likewise for other functions.

The convex and Lipschitz continuous Fischer-Burmeister function $\varphi : \mathbb{R}^2 \to \mathbb{R}$ is defined by

$$\varphi(a,b) := \sqrt{a^2 + b^2} - a - b, \tag{13}$$

cf. Fischer [6]. The Fischer-Burmeister function has the nice property that $\varphi(a,b) = 0$ holds if and only if $a, b \geq 0$ and $ab = 0$. Hence, the complementarity conditions (12) are equivalent with the equality

$$\varphi(-c_i(x_*(t), y_*(t), u_*(t)), \eta_{i,*}(t)) = 0, \qquad i = 1, \ldots, n_c,$$

that has to hold almost everywhere in $[0,1]$. Rather than working with the derivative of φ, which does not exist at the origin, we will work with Clarke's generalized Jacobian of φ:

$$\partial\varphi(a,b) = \begin{cases} \left\{\left(\dfrac{a}{\sqrt{a^2+b^2}} - 1, \dfrac{b}{\sqrt{a^2+b^2}} - 1\right)\right\}, & \text{if } (a,b) \neq (0,0), \\ \left\{(s,r) \;\middle|\; (s+1)^2 + (r+1)^2 \leq 1\right\}, & \text{if } (a,b) = (0,0). \end{cases}$$

Notice, that $\partial\varphi(a,b)$ is a nonempty, convex and compact set. For $1 \leq r \leq \infty$ let the Banach spaces

$$\begin{aligned} Z_r &= W^{1,r}([0,1],\mathbb{R}^{n_x}) \times L^r([0,1],\mathbb{R}^{n_y}) \times L^r([0,1],\mathbb{R}^{n_u}) \\ &\quad \times W^{1,r}([0,1],\mathbb{R}^{n_x}) \times L^r([0,1],\mathbb{R}^{n_y}) \times L^r([0,1],\mathbb{R}^{n_c}) \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_\psi}, \\ Y_{1,r} &= L^r([0,1],\mathbb{R}^{n_x}) \times W^{1,r}([0,1],\mathbb{R}^{n_y}) \times L^r([0,1],\mathbb{R}^{n_x}) \times L^r([0,1],\mathbb{R}^{n_y}) \\ &\quad \times \mathbb{R}^{n_\psi} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \times L^r([0,1],\mathbb{R}^{n_u}), \\ Y_{2,r} &= L^r([0,1],\mathbb{R}^{n_c}) \end{aligned}$$

be equipped with the maximum norm for product spaces and $z_* = (x_*, y_*, u_*, \lambda_{f,*}, \lambda_{g,*}, \eta_*, \zeta_*, \sigma_*)$. Then, the necessary conditions (4)-(12) are equivalent with the nonlinear equation

$$F(z_*) = \begin{pmatrix} F_1(z_*) \\ F_2(z_*) \end{pmatrix} = 0, \tag{14}$$

where $F_1 : Z_\infty \to Y_{1,r}$ and $F_2 : Z_\infty \to Y_{2,r}$ denote the smooth and the nonsmooth part of $F : Z_\infty \to Y_r := Y_{1,r} \times Y_{2,r}$ with $1 \leq r \leq \infty$, respectively:

$$F_1(z)(\cdot) := \begin{pmatrix} x'(\cdot) - f(x(\cdot), y(\cdot), u(\cdot)) \\ g(x(\cdot)) \\ \lambda_f'(\cdot) + H_x'(x(\cdot), y(\cdot), u(\cdot), \lambda_f(\cdot), \lambda_g(\cdot), \eta(\cdot))^\top \\ H_y'(x(\cdot), y(\cdot), u(\cdot), \lambda_f(\cdot), \lambda_g(\cdot), \eta(\cdot))^\top \\ \psi(x(0), x(1)) \\ \lambda_f(0) + \psi_{x_0}'(x(0), x(1))^\top \sigma + g_x'(x(0))^\top \zeta \\ \lambda_f(1) - \psi_{x_1}'(x(0), x(1))^\top \sigma \\ H_u'(x(\cdot), y(\cdot), u(\cdot), \lambda_f(\cdot), \lambda_g(\cdot), \eta(\cdot))^\top \end{pmatrix}, \tag{15}$$

$$F_2(z)(\cdot) := \omega(z(\cdot)), \tag{16}$$

where $\omega = (\omega_1, \ldots, \omega_{n_c})^\top : \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_c} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_\psi} \to \mathbb{R}^{n_c}$ and

$$\omega_i(\bar{x}, \bar{y}, \bar{u}, \bar{\lambda}_f, \bar{\lambda}_g, \bar{\eta}, \bar{\zeta}, \bar{\sigma}) := \varphi(-c_i(\bar{x}, \bar{y}, \bar{u}), \bar{\eta}_i), \qquad i = 1, \ldots, n_c. \tag{17}$$

For technical reasons, which become apparent later, we consider F as a mapping from Z_∞ into Y_r. However, we note that

$$\operatorname{im}(F) \subseteq Y_\infty \subset Y_r \quad \text{for every } 1 \leq r < \infty.$$

Notice, that the first component F_1 of F in (15) as a mapping from Z_∞ to $Y_{1,\infty}$ is continuously Fréchet-differentiable with

$$F_1'(z^k)(z) = \begin{pmatrix} x' - f_x'x - f_y'y - f_u'u \\ g_x'x \\ \lambda_f' + H_{xx}''x + H_{xy}''y + H_{xu}''u + H_{x\lambda_f}''\lambda_f + H_{x\lambda_g}''\lambda_g + H_{x\eta}''\eta \\ H_{yx}''x + H_{yy}''y + H_{yu}''u + H_{y\lambda_f}''\lambda_f + H_{y\lambda_g}''\lambda_g + H_{y\eta}''\eta \\ \psi_{x_0}'x(0) + \psi_{x_1}'x(1) \\ \lambda_f(0) + ({\psi_{x_0}'}^\top\sigma^k + {g_x'}^\top\zeta^k)_{x_0}'x(0) + ({\psi_{x_0}'}^\top\sigma^k)_{x_1}'x(1) + {\psi_{x_0}'}^\top\sigma + {g_x'}^\top\zeta \\ \lambda_f(1) - ({\psi_{x_1}'}^\top\sigma^k)_{x_0}'x(0) - ({\psi_{x_1}'}^\top\sigma^k)_{x_1}'x(1) - {\psi_{x_1}'}^\top\sigma \\ H_{ux}''x + H_{uy}''y + H_{uu}''u + H_{u\lambda_f}''\lambda_f + H_{u\lambda_g}''\lambda_g + H_{u\eta}''\eta \end{pmatrix}$$

provided that the functions f_0, f, g, c, ψ are twice continuously differentiable w.r.t. all arguments. All functions are evaluated at $z^k = (x^k, y^k, u^k, \lambda_f^k, \lambda_g^k, \eta^k, \zeta^k, \sigma^k) \in Z_\infty$. The Fréchet differentiability from Z_∞ to $Y_{1,\infty}$ implies that F_1 is continuously Fréchet-differentiable as a mapping from Z_∞ to $Y_{1,r}$ for every $1 \le r \le \infty$, because

$$\begin{aligned} &\lim_{\|h\|_{Z_\infty}\to 0} \frac{\|F_1(z+h) - F_1(z) - F_1'(z)(h)\|_{Y_r}}{\|h\|_{Z_\infty}} \\ \le &\lim_{\|h\|_{Z_\infty}\to 0} \frac{C\,\|F_1(z+h) - F_1(z) - F_1'(z)(h)\|_{Y_\infty}}{\|h\|_{Z_\infty}} = 0, \end{aligned}$$

where $C > 0$ is a constant.

The standard approach to solve (14) numerically would be to apply the classical Newton's method. Unfortunately, the derivative $F'(z^k)$ does not exist since the component F_2 is not differentiable. Motivated by Clarke's generalized Jacobian and the chain rule for non-smooth functions in finite dimensions, see Clarke [5], we define the point to set mapping $\partial_* F : Z \rightrightarrows \mathcal{L}(Z_r, Y_r)$ according to

$$\partial_* F(z^k)(z) := \left\{ \begin{pmatrix} F_1'(z^k)(z) \\ -S\left(c_x'[\cdot]x + c_y'[\cdot]y + c_u'[\cdot]u\right) + R\eta \end{pmatrix} \;\middle|\; \begin{array}{l} S = diag(s_1, \ldots, s_{n_c}), \\ R = diag(r_1, \ldots, r_{n_c}), \\ (s_i, r_i) \in \partial\varphi[\cdot] \text{ a.e.}, \\ s_i(\cdot), r_i(\cdot) \text{ measurable} \end{array} \right\}$$

and use this set as a generalized Jacobian. The same idea was introduced earlier in Ulbrich [30], Def. 3.35, p. 47, and Gerdts [13].

It is straightforward to show that every $V \in \partial_* F(z^k)$ defines a linear and bounded operator from Z_r into Y_r for every $1 \le r \le \infty$.

Replacing the non-existing Jacobian F' in the classical Newton's method by the generalized Jacobian $\partial_* F(z^k)$ leads to the following algorithm. The algorithm makes use of a smoothing operator $S_k : Z_r \to Z_\infty$, see Ulbrich [30], which maps $z^k + d^k \in Z_r$ back to Z_∞. However, we shall see later that the smoothing step is not necessary in our setting as under suitable assumptions V_k^{-1} maps Y_∞ onto Z_∞ and thus $d^k \in Z_\infty$ holds whenever $F(z^k) \in Y_\infty$, which in turn holds true whenever $z^k \in Z_\infty$.

Algorithm 1 (Local Semi-Smooth Newton's Method)

(0) Choose z^0.
(1) If some stopping criterion is satisfied, stop.
(2) Choose an arbitrary $V_k \in \partial_* F(z^k)$ and compute the search direction d^k from the linear equation

$$V_k(d^k) = -F(z^k).$$

(3) Set $z^{k+1} = S_k(z^k + d^k)$, $k = k+1$, and goto (1).

The assumptions needed to prove local convergence of the method are similar to those in Qi [24], Qi and Sun [25], Jiang [17], and Ulbrich [30]. $\partial_* F(z)$ is called nonsingular if for every $V \in \partial_* F(z)$ the inverse operator V^{-1} exists and if it is linear and bounded, i.e. $V^{-1} \in \mathcal{L}(Y_r, Z_r)$.

Theorem 1 *Let $z_* \in Z_\infty$ be a zero of F. Suppose that there exist constants $\Delta > 0$, $C > 0$, and $1 \le r \le \infty$ such that for every $\|z - z_*\|_{Z_\infty} < \Delta$ the generalized Jacobian $\partial_* F(z)$ of the mapping $F : Z_\infty \to Y_r$ is nonsingular and $\|V^{-1}\|_{\mathcal{L}(Y_r,Z_r)} \le C$ for every $V \in \partial_* F(z)$. Moreover, let there exist a constant $C_S > 0$ such that*

$$\|S_k(z^k + d^k) - z_*\|_{Z_\infty} \le C_S \|z^k + d^k - z_*\|_{Z_r}$$

for all k.

Moreover, let F be semi-smooth, compare Ulbrich [30], Def. 3.1, p. 34:

$$\sup_{V \in \partial_* F(z)} \|F(z) - F(z_*) - V(z - z_*)\|_{Y_r} = o(\|z - z_*\|_{Z_\infty}) \quad \text{as } \|z - z_*\|_{Z_\infty} \to 0.$$

Then, for z^0 sufficiently close to z_* the semi-smooth Newton's method converges superlinearly to z_*.

Furthermore, if $F(z^k) \neq 0$ for all k and if there is a constant $\tilde{C}_S$ with $\|S_k(z^k + d^k) - z^k\|_{Z_\infty} \le \tilde{C}_S \cdot \|d^k\|_{Y_r}$ for every k, then the residual values converge superlinearly:

$$\lim_{k\to\infty} \frac{\|F(z^{k+1})\|_{Y_r}}{\|F(z^k)\|_{Y_r}} = 0.$$

Proof Due to the first assumption, the algorithm is well-defined in some neighborhood of z_*. It holds

$$V_k(z^k + d^k - z_*) = V_k(z^k - z_*) + V_k d^k = V_k(z^k - z_*) - F(z^k) + F(z_*).$$

The first assertion follows from

$$
\begin{aligned}
\|z^{k+1} - z_*\|_{Z_\infty} &= \|S_k(z^k + d^k) - z_*\|_{Z_\infty} &(18)\\
&\le C_S \cdot \|z^k + d^k - z_*\|_{Z_r} &(19)\\
&= C_S \cdot \|V_k^{-1}\left(V_k(z^k - z_*) - F(z^k) + F(z_*)\right)\|_{Z_r}\\
&\le C_S \cdot \|V_k^{-1}\|_{\mathcal{L}(Y_r,Z_r)} \cdot \|F(z^k) - F(z_*) - V_k(z^k - z_*)\|_{Y_r}\\
&\le C_S \cdot C \cdot \|F(z^k) - F(z_*) - V_k(z^k - z_*)\|_{Y_r}\\
&= \begin{cases} o(\|z^k - z_*\|_{Z_\infty}), & \text{in case (i),}\\ \mathcal{O}(\|z^k - z_*\|_{Z_\infty}^{1+p}), & \text{in case (ii).}\end{cases} &(20)
\end{aligned}
$$

Let $\varepsilon > 0$ be arbitrary. According to Equation (20) there exists $\delta > 0$ with

$$\|z^{k+1} - z_*\|_{Z_\infty} \le \varepsilon\|z^k - z_*\|_{Z_\infty} \quad \text{whenever} \quad \|z^k - z_*\|_{Z_\infty} \le \delta.$$

Notice, that for any $\delta > 0$ there exists some $k_0(\delta)$ such that $\|z^k - z_*\|_{Z_\infty} \le \delta$ for every $k \ge k_0(\delta)$ since z^k converges to z_*. By the local Lipschitz continuity of F we get

$$\|F(z^{k+1})\|_{Y_r} = \|F(z^{k+1}) - F(z_*)\|_{Y_r} \le L\|z^{k+1} - z_*\|_{Z_\infty} \le L\varepsilon\|z^k - z_*\|_{Z_\infty}$$

locally around z_* and the Newton iteration implies

$$\|z^{k+1} - z^k\|_{Z_\infty} \le \tilde{C}_S \cdot \|V_k^{-1}\|_{\mathcal{L}(Y_r,Z_r)} \cdot \|F(z^k)\|_{Y_r} \le \tilde{C}_S \cdot C \cdot \|F(z^k)\|_{Y_r}.$$

Thus,

$$
\begin{aligned}
\|z^k - z_*\|_{Z_\infty} &\le \|z^{k+1} - z^k\|_{Z_\infty} + \|z^{k+1} - z_*\|_{Z_\infty}\\
&\le \tilde{C}_S \cdot C \cdot \|F(z^k)\|_{Y_r} + \|z^{k+1} - z_*\|_{Z_\infty}\\
&\le \tilde{C}_S \cdot C \cdot \|F(z^k)\|_{Y_r} + \varepsilon\|z^k - z_*\|_{Z_\infty}
\end{aligned}
$$

and

$$\|z^k - z_*\|_{Z_\infty} \le \frac{\tilde{C}_S \cdot C}{1-\varepsilon}\|F(z^k)\|_{Y_r}.$$

Finally,

$$\|F(z^{k+1})\|_{Y_r} \le L\varepsilon\|z^k - z_*\|_{Z_\infty} \le \frac{L\varepsilon\tilde{C}_S C}{1-\varepsilon}\|F(z^k)\|_{Y_r}.$$

Since $F(z^k) \ne 0$ and ε may be arbitrarily small this shows the last assertion.

Remark 1 In the above theorem it suffices if the assumptions are satisfied for certain elements of $\partial_* F$ provided that only these elements are used in the algorithm. For the upcoming computations we used the element corresponding to the choices

$$
\begin{aligned}
s_i(t) &= \begin{cases} -1, & \text{if } c_i[t] = 0,\ \eta_i(t) = 0,\\ \frac{-c_i[t]}{\sqrt{c_i[t]^2 + \eta_i(t)^2}} - 1, & \text{otherwise,}\end{cases}\\
r_i(t) &= \begin{cases} 0, & \text{if } c_i[t] = 0,\ \eta_i(t) = 0,\\ \frac{\eta(t)}{\sqrt{c_i[t]^2 + \eta_i(t)^2}} - 1, & \text{otherwise.}\end{cases}
\end{aligned}
$$

For $1 \leq r < \infty$ the operator F turns out to be semi-smooth and we obtain the following local convergence result:

Theorem 2 *Let $z_* \in Z_\infty$ be a zero of F. Let $1 \leq r < \infty$. Suppose that there exist constants $\Delta > 0$ and $C > 0$ such that for every $\|z - z_*\|_{Z_\infty} < \Delta$ the generalized Jacobian $\partial_* F(z)$ of the mapping $F : Z_\infty \to Y_r$ is nonsingular and $\|V^{-1}\|_{\mathcal{L}(Y_r, Z_r)} \leq C$ for every $V \in \partial_* F(z)$. Moreover, let there exist a constant $C_S > 0$ such that*

$$\|S_k(z^k + d^k) - z_*\|_{Z_\infty} \leq C_S \|z^k + d^k - z_*\|_{Z_r}$$

for all k.

Then, the semismooth Newton method converges locally at a superlinear rate, if f_0, f, g, c, ψ are twice continuously differentiable.

Furthermore, if $F(z^k) \neq 0$ for all k and if there is a constant $\tilde{C}_S$ with $\|S_k(z^k + d^k) - z^k\|_{Z_\infty} \leq \tilde{C}_S \cdot \|d^k\|_{Y_r}$ for every k, then the residual values converge superlinearly:

$$\lim_{k \to \infty} \frac{\|F(z^{k+1})\|_{Y_r}}{\|F(z^k)\|_{Y_r}} = 0.$$

Proof We need to show that the operator $F : Z_\infty \to Y_r$ is semismooth for every $1 \leq r < \infty$.

As F_1 is continuously Fréchet-differentiable as a mapping from Z_∞ to Y_r for every $1 \leq r \leq \infty$ if f_0, f, g, c, ψ are twice continuously differentiable, the component F_1 is semismooth.

The second component $F_2(z)(t) = \omega(z(t))$ of F is a superposition operator as in Ulbrich [30], Sec. 3.3, which maps L^∞ into L^r. It was shown in Ulbrich [30], Theorems 3.44 and 3.48, that the superposition operator F_2 is semismooth as a mapping from Z_∞ to $Y_{2,r}$ for every $1 \leq r < \infty$, if the following assumptions are satisfied:

- The operator $G : Z_\infty \to Y_{2,r}$, $1 \leq r < \infty$, defined by

$$G(z)(\cdot) = (c(x(\cdot), y(\cdot), u(\cdot)), \eta(\cdot))$$

  is continuously Fréchet differentiable.
- The mapping $z \in Z_\infty \mapsto G(z) \in Y_{2,\infty}$ is locally Lipschitz continuous.
- φ is Lipschitz continuous and semismooth.

Please note that $r = \infty$ is excluded.

The Fischer-Burmeister function $\varphi : \mathbb{R}^2 \to \mathbb{R}$ is Lipschitz continuous and semismooth, see Fischer [7], Lemma 20. The mapping $z \in Z_\infty \mapsto G(z) \in Y_{2,\infty}$ is continuously Fréchet differentiable (and thus locally Lipschitz continuous), if c is continuously differentiable. This implies that the operator G as a mapping from Z_∞ to $Y_{2,r}$ for every $1 \leq r < \infty$ is continuously Fréchet differentiable. Hence, the operator F_2 is semismooth as an operator from Z_∞ to $Y_{2,r}$ with $1 \leq r < \infty$. Theorem 1 completes the proof.

The crucial assumption in Theorem 2 is the non-singularity of $\partial_* F(z)$ and the uniform boundedness of V^{-1} for every $V \in \partial_* F(z)$. In the next section sufficient conditions for these assumptions are presented.

3 Computation of the Search Direction and Uniform Non-Singularity

For brevity we neglect the arguments whenever possible. The linear operator equation $V_k(d^k) = -F(z^k)$ in step (2) of Algorithm 1 reads as

$$\begin{pmatrix} x' \\ \lambda_f' \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} - \begin{pmatrix} f_x' & 0 & f_y' & 0 & f_u' & 0 \\ -H_{xx}'' & -H_{x\lambda_f}'' & -H_{xy}'' & -H_{x\lambda_g}'' & -H_{xu}'' & -H_{x\eta}'' \\ -g_x' & 0 & 0 & 0 & 0 & 0 \\ -H_{yx}'' & -H_{y\lambda_f}'' & -H_{yy}'' & -H_{y\lambda_g}'' & -H_{yu}'' & -H_{y\eta}'' \\ -H_{ux}'' & -H_{u\lambda_f}'' & -H_{uy}'' & -H_{u\lambda_g}'' & -H_{uu}'' & -H_{u\eta}'' \\ Sc_x' & 0 & Sc_y' & 0 & Sc_u' & -R \end{pmatrix} \begin{pmatrix} x \\ \lambda_f \\ y \\ \lambda_g \\ u \\ \eta \end{pmatrix} = - \begin{pmatrix} (x^k)' - f \\ (\lambda_f^k)' + (H_x')^\top \\ g \\ (H_y')^\top \\ (H_u')^\top \\ \omega(z^k(\cdot)) \end{pmatrix} \tag{21}$$

and

$$\begin{pmatrix} \psi_{x_0}' & 0 & 0 & 0 \\ ({\psi_{x_0}'}^\top \sigma^k + {g_x'}^\top \zeta^k)_{x_0}' & I & {g_x'}^\top & {\psi_{x_0}'}^\top \\ -({\psi_{x_1}'}^\top \sigma^k)_{x_0}' & 0 & 0 & -{\psi_{x_1}'}^\top \end{pmatrix} \begin{pmatrix} x(0) \\ \lambda_f(0) \\ \zeta \\ \sigma \end{pmatrix} + \begin{pmatrix} \psi_{x_1}' & 0 & 0 & 0 \\ ({\psi_{x_0}'}^\top \sigma^k)_{x_1}' & 0 & 0 & 0 \\ -({\psi_{x_1}'}^\top \sigma^k)_{x_1}' & I & 0 & 0 \end{pmatrix} \begin{pmatrix} x(1) \\ \lambda(1) \\ \zeta \\ \sigma \end{pmatrix} = - \begin{pmatrix} \psi(x^k(0), x^k(1)) \\ \lambda_f^k(0) + {\psi_{x_0}'}^\top \sigma^k + {g_x'}^\top \zeta^k \\ \lambda_f^k(1) - {\psi_{x_1}'}^\top \sigma^k \end{pmatrix}. \tag{22}$$

Herein, every function is evaluated at the current iterate z^k. We analyze properties of this DAE. Equations (21) and (22) can be written as

$$\begin{pmatrix} x' \\ \lambda_f' \\ 0 \\ 0 \end{pmatrix} - \begin{pmatrix} f_x' & 0 & f_y' & 0 \\ -H_{xx}'' & -H_{x\lambda_f}'' & -H_{xy}'' & -H_{x\lambda_g}'' \\ -g_x' & 0 & 0 & 0 \\ -H_{yx}'' & -H_{y\lambda_f}'' & -H_{yy}'' & -H_{y\lambda_g}'' \end{pmatrix} \begin{pmatrix} x \\ \lambda_f \\ y \\ \lambda_g \end{pmatrix} - \begin{pmatrix} f_u' & 0 \\ -H_{xu}'' & -H_{x\eta}'' \\ 0 & 0 \\ -H_{yu}'' & -H_{y\eta}'' \end{pmatrix} \begin{pmatrix} u \\ \eta \end{pmatrix} = - \begin{pmatrix} (x^k)' - f \\ (\lambda_f^k)' + (H_x')^\top \\ g \\ (H_y')^\top \end{pmatrix} \tag{23}$$

and

$$\begin{pmatrix} \psi'_{x_0} & 0 & 0 & 0 \\ ({\psi'_{x_0}}^\top \sigma^k + {g'_x}^\top \zeta^k)'_{x_0} & I & {g'_x}^\top & {\psi'_{x_0}}^\top \\ -({\psi'_{x_1}}^\top \sigma^k)'_{x_0} & 0 & 0 & -{\psi'_{x_1}}^\top \end{pmatrix} \begin{pmatrix} x(0) \\ \lambda_f(0) \\ \zeta \\ \sigma \end{pmatrix}$$

$$+ \begin{pmatrix} \psi'_{x_1} & 0 \; 0 \; 0 \\ ({\psi'_{x_0}}^\top \sigma^k)'_{x_1} & 0 \; 0 \; 0 \\ -({\psi'_{x_1}}^\top \sigma^k)'_{x_1} & I \; 0 \; 0 \end{pmatrix} \begin{pmatrix} x(1) \\ \lambda(1) \\ \zeta \\ \sigma \end{pmatrix} = - \begin{pmatrix} \psi(x^k(0), x^k(1)) \\ \lambda^k_f(0) + {\psi'_{x_0}}^\top \sigma^k + {g'_x}^\top \zeta^k \\ \lambda^k_f(1) - {\psi'_{x_1}}^\top \sigma^k \end{pmatrix}, \tag{24}$$

and

$$\mathcal{A} \begin{pmatrix} u \\ \eta \end{pmatrix} + \begin{pmatrix} H''_{ux} & H''_{u\lambda_f} & H''_{uy} & H''_{u\lambda_g} \\ -Sc'_x & 0 & -Sc'_y & 0 \end{pmatrix} \begin{pmatrix} x \\ \lambda_f \\ y \\ \lambda_g \end{pmatrix} = - \begin{pmatrix} (H'_u)^\top \\ \omega(z^k(\cdot)) \end{pmatrix}, \tag{25}$$

where

$$\mathcal{A} := \begin{pmatrix} H''_{uu} & (c'_u)^\top \\ -Sc'_u & R \end{pmatrix}. \tag{26}$$

Herein, every function is evaluated at the current iterate z^k. If the inverse operator $\mathcal{A}^{-1}$ exists, equation (25) can be solved for u and η according to

$$\begin{pmatrix} u \\ \eta \end{pmatrix} = -\mathcal{A}^{-1} \left[\begin{pmatrix} H''_{ux} & H''_{u\lambda_f} & H''_{uy} & H''_{u\lambda_g} \\ -Sc'_x & 0 & -Sc'_y & 0 \end{pmatrix} \begin{pmatrix} x \\ \lambda_f \\ y \\ \lambda_g \end{pmatrix} + \begin{pmatrix} (H'_u)^\top \\ \omega(z^k(\cdot)) \end{pmatrix} \right], \tag{27}$$

which means u and η are so-called index-1 variables. The constants σ and ζ can be viewed as solutions of the differential equations $\sigma' = 0$ and $\zeta' = 0$. Introducing (27) into the differential-algebraic equation (23), augmenting this system by $\sigma' = 0$ and $\zeta' = 0$, and taking into account the boundary conditions (24), yields the linear DAE boundary value problem for the differential variable $\xi = (x, \lambda_f, \sigma, \zeta)^\top$, the index-2 algebraic variable y and the index-1 algebraic variable λ_g.

$$\xi' = B_d\xi + B_1\lambda_g + B_2 y + b, \tag{28}$$

$$0 = G_d\xi + g, \tag{29}$$

$$0 = F_d\xi + \tilde{F}_1\lambda_g + \tilde{F}_2 y + \tilde{f}, \tag{30}$$

$$q = E_0\xi(0) + E_1\xi(1), \tag{31}$$

where

$$
\begin{aligned}
B_d &= \begin{pmatrix} f'_x & 0 & 0\;0 \\ -H''_{xx} & -H''_{x\lambda_f} & 0\;0 \\ 0 & 0 & 0\;0 \\ 0 & 0 & 0\;0 \end{pmatrix} - \begin{pmatrix} f'_u & 0 \\ -H''_{xu} & -H''_{x\eta} \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \mathcal{A}^{-1} \begin{pmatrix} H''_{ux} & H''_{u\lambda_f} & 0\;0 \\ -Sc'_x & 0 & 0\;0 \end{pmatrix}, \\
B_1 &= \begin{pmatrix} 0 \\ -H''_{x\lambda_g} \\ 0 \\ 0 \end{pmatrix} - \begin{pmatrix} f'_u & 0 \\ -H''_{xu} & -H''_{x\eta} \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \mathcal{A}^{-1} \begin{pmatrix} H''_{u\lambda_g} \\ 0 \end{pmatrix}, \\
B_2 &= \begin{pmatrix} f'_y \\ -H''_{xy} \\ 0 \\ 0 \end{pmatrix} - \begin{pmatrix} f'_u & 0 \\ -H''_{xu} & -H''_{x\eta} \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \mathcal{A}^{-1} \begin{pmatrix} H''_{uy} \\ -Sc'_y \end{pmatrix}, \\
b &= -\begin{pmatrix} (x^k)' - f \\ (\lambda_f^k)' + (H'_x)^\top \\ 0 \\ 0 \end{pmatrix} - \begin{pmatrix} f'_u & 0 \\ -H''_{xu} & -H''_{x\eta} \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \mathcal{A}^{-1} \begin{pmatrix} (H'_u)^\top \\ \omega(z^k(\cdot)) \end{pmatrix}, \\
G_d &= \begin{pmatrix} g'_x & 0 & 0 & 0 \end{pmatrix}, \\
F_d &= \begin{pmatrix} -H''_{yx} & -H''_{y\lambda_f} & 0\;0 \end{pmatrix} - \begin{pmatrix} -H''_{yu} & -H''_{y\eta} \end{pmatrix} \mathcal{A}^{-1} \begin{pmatrix} H''_{ux} & H''_{u\lambda_f} & 0\;0 \\ -Sc'_x & 0 & 0\;0 \end{pmatrix}, \\
\tilde{F}_1 &= -H''_{y\lambda_g} - \begin{pmatrix} -H''_{yu} & -H''_{y\eta} \end{pmatrix} \mathcal{A}^{-1} \begin{pmatrix} H''_{u\lambda_g} \\ 0 \end{pmatrix}, \\
\tilde{F}_2 &= -H''_{yy} - \begin{pmatrix} -H''_{yu} & -H''_{y\eta} \end{pmatrix} \mathcal{A}^{-1} \begin{pmatrix} H''_{uy} \\ -Sc'_y \end{pmatrix}, \\
\tilde{f} &= -\left(H'_y\right)^\top - \begin{pmatrix} -H''_{yu} & -H''_{y\eta} \end{pmatrix} \mathcal{A}^{-1} \begin{pmatrix} (H'_u)^\top \\ \omega(z^k(\cdot)) \end{pmatrix}, \\
E_0 &= \begin{pmatrix} \psi'_{x_0} & 0 & 0 & 0 \\ ({\psi'_{x_0}}^\top \sigma^k + {g'_x}^\top \zeta^k)'_{x_0} & I & {g'_x}^\top & {\psi'_{x_0}}^\top \\ -({\psi'_{x_1}}^\top \sigma^k)'_{x_0} & 0 & 0 & -{\psi'_{x_1}}^\top \end{pmatrix}, \\
E_1 &= \begin{pmatrix} \psi'_{x_1} & 0\;0\;0 \\ ({\psi'_{x_0}}^\top \sigma^k)'_{x_1} & 0\;0\;0 \\ -({\psi'_{x_1}}^\top \sigma^k)'_{x_1} & I\;0\;0 \end{pmatrix}, \\
q &= -\begin{pmatrix} \psi(x^k(0), x^k(1)) \\ \lambda_f^k(0) + {\psi'_{x_0}}^\top \sigma^k + {g'_x}^\top \zeta^k \\ \lambda_f^k(1) - {\psi'_{x_1}}^\top \sigma^k \end{pmatrix}.
\end{aligned}
$$

A sufficient condition for the existence of the inverse operator $\mathcal{A}^{-1}$ was established in Gerdts [13], Theorem 3.2.

Theorem 3 *Let $z = (x, y, u, \lambda_f, \lambda_g, \eta, \zeta, \sigma) \in Z_\infty$ be given. Define the index sets*

$$
\begin{aligned}
I_>(t) &:= \{i \in \{1, \ldots, n_c\} \mid c_i[t] = 0,\ \eta_i(t) > 0\}, \\
J_\gamma(t) &:= \{i \in \{1, \ldots, n_c\} \mid |c_i[t]| \le \gamma \eta_i(t),\ \eta_i(t) \ge 0\}, \qquad \gamma > 0.
\end{aligned}
$$

Let the following assumptions hold at z:

(i) *Let there exist constants* C_1, C_2, C_3 *such that a.e. in* $[0,1]$ *it holds*

$$\|H''_{uu}[t]\| \leq C_1, \quad \|c'_u[t]^\top\| \leq C_2, \quad \|c'_u[t]\| \leq C_3.$$

(ii) *(Coercivity) Let there exist a constant* $\alpha > 0$ *such that a.e. in* $[0,1]$ *it holds*

$$d^\top H''_{uu}[t]d \geq \alpha\|d\|^2 \quad \text{for all} \quad d \in \mathbb{R}^{n_u} \ : \ c'_{I_>(t),u}[t]d = 0.$$

(iii) *(Linear independence) Let there exist constants* $\gamma > 0$ *and* $\beta > 0$ *such that a.e. in* $[0,1]$ *it holds*

$$\|c'_{J_\gamma(t),u}[t]^\top\zeta\| \geq \beta\|\zeta\| \quad \text{for all } \zeta \text{ of appropriate dimension.}$$

Then, a.e. in $[0,1]$ *the inverse operator* $\mathcal{A}^{-1}(t)$ *exists and it holds* $\|\mathcal{A}^{-1}(t)\| \leq C$ *for some constant* C.

We need an auxiliary result.

Lemma 1 *Consider the linear BVP (28)-(31).*

Let there exist a constant C *such that a.e. in* $[0,1]$ $\tilde{F}_1(t)$ *is nonsingular and* $\|\tilde{F}_1^{-1}(t)\| \leq C$.

Then, a.e. in $[0,1]$ *it holds*

$$\lambda_g(t) = -\tilde{F}_1(t)^{-1}\left(F_d(t)\xi(t) + \tilde{F}_2(t)y(t) + \tilde{f}(t)\right)$$

and

$$\|\lambda_g\|_\infty \leq C\left(\|F_d\|_\infty\|\xi\|_{1,\infty} + \|\tilde{F}_2\|_\infty\|y\|_\infty + \|\tilde{f}\|_\infty\right)$$

Moreover, the BVP (28)-(31) reduces to the linear BVP

$$\xi' = \hat{B}_d\xi + \hat{B}_2 y + \hat{b}, \tag{32}$$

$$0 = G_d\xi + g, \tag{33}$$

$$q = E_0\xi(0) + E_1\xi(1), \tag{34}$$

where

$$\hat{B}_d = B_d - B_1\tilde{F}_1^{-1}F_d, \quad \hat{B}_2 = B_2 - B_1\tilde{F}_1^{-1}\tilde{F}_2, \quad \hat{b} = b - B_1\tilde{F}_1^{-1}\tilde{f}.$$

Proof. Solve (30) for λ_g and introduce it into (28).

It remains to establish the non-singularity and the boundedness of the inverse of the linear operator defining the BVP (32)-(34). This operator $T : \Omega_0 \to \Omega_1$, $\Omega_0 := W^{1,r}([0,1], \mathbb{R}^{2n_x+n_\psi+n_y}) \times L^r([0,1], \mathbb{R}^{n_y})$, $\Omega_1 := L^r([0,1], \mathbb{R}^{2n_x+n_\psi+n_y}) \times W^{1,r}([0,1], \mathbb{R}^{n_y}) \times \mathbb{R}^{2n_x+n_\psi}$ is defined by

$$T(\xi, y)(t) = \begin{pmatrix} \xi'(t) - \hat{B}_d(t)\xi(t) - \hat{B}_2(t)y(t) \\ G_d(t)\xi(t) \\ E_0\xi(0) + E_1\xi(1) \end{pmatrix}$$

with $\|(\xi, y)\|_{\Omega_0} = \max\{\|\xi\|_{1,r}, \|y\|_r\}$ and $\|(\omega_1, \omega_2, \omega_3)\|_{\Omega_1} = \max\{\|\omega_1\|_r, \|\omega_2\|_{1,r}, \|\omega_3\|\}$.

Theorem 4 *Consider the operator equation $T(\xi, y) = (\omega_1, \omega_2, \omega_3)^\top$. Let the following assumptions be satisfied:*

(i) Let there exist a constant C such that a.e. in $[0,1]$ it holds

$$\|\hat{B}_d(t)\|, \|\hat{B}_2(t)\|, \|G_d(t)\|, \|G_d'(t)\|, \|\hat{b}(t)\|, \|g(t)\| \leq C.$$

(ii) Let there exist a constant C_1 such that a.e. in $[0,1]$ $M := G_d\hat{B}_2$ is nonsingular and $\|M(t)^{-1}\| \leq C_1$.

(iii) Let there exist $\kappa > 0$ such that for all $\mu \in \mathbb{R}^{2n_x+n_\psi}$ it holds

$$\| \left(E_0\Phi(0) + E_1\Phi(1)\right) \Gamma\mu\| \geq \kappa\|\mu\|,$$

where Φ is a fundamental solution with $\Phi'(t) = B(t)\Phi(t)$, $\Phi(0) = I$ and Γ is defined in (a) below.

Define

$$\begin{aligned}
B(t) &:= \hat{B}_d(t) - \hat{B}_2(t)M(t)^{-1}Q(t),\\
\omega(t) &:= \omega_1(t) - \hat{B}_2(t)M(t)^{-1}q(t),\\
Q(t) &:= G_d'(t) + G_d(t)\hat{B}_d(t),\\
q(t) &:= -\omega_2'(t) + G_d(t)\omega_1(t).
\end{aligned}$$

Then:

(a) There exist consistent initial values $\xi(0) = \xi_0$ satisfying $0 = G_d(0)\xi_0 - \omega_2(0)$ and every consistent ξ_0 possesses the representation

$$\xi_0 = \Pi\omega_2(0) + \Gamma\mu,$$

where $\Pi \in \mathbb{R}^{(2n_x+n_\psi+n_y)\times n_y}$ satisfies $(I - G_d(0)\Pi)\omega_2(0) = 0$ and the columns of $\Gamma \in \mathbb{R}^{(2n_x+n_\psi+n_y)\times(2n_x+n_\psi)}$ define an orthonormal basis of $ker(G_d(0))$, i.e. $G_d(0)\Gamma = 0$. Vice versa, every such ξ_0 is consistent for arbitrary $\mu \in \mathbb{R}^{2n_x+n_\psi}$.

(b) The initial value problem

$$\begin{aligned}
\xi'(t) - \hat{B}_d(t)\xi(t) - \hat{B}_2(t)y(t) &= \omega_1(t),\\
G_d(t)\xi(t) &= \omega_2(t),
\end{aligned}$$

together with the consistent initial value $\xi(0) = \xi_0 = \Pi\omega_2(0) + \Gamma\mu$ has a unique solution $\xi(\cdot) \in W^{1,r}([0,1], \mathbb{R}^{2n_x+n_\psi+n_y})$, for every $\mu \in \mathbb{R}^{2n_x+n_\psi}$, every $\omega_1(\cdot) \in L^r([0,1], \mathbb{R}^{2n_x+n_\psi+n_y})$ and every $\omega_2(\cdot) \in W^{1,r}([0,1], \mathbb{R}^{n_y})$. The solution is given by

$$\xi(t) = \Phi(t)\left(\Pi\omega_2(0) + \Gamma\mu + \int_0^t \Phi^{-1}(\tau)\omega(\tau)d\tau\right) \qquad \text{in } [0,1], \tag{35}$$

$$y(t) = -M(t)^{-1}\left(q(t) + Q(t)\xi(t)\right) \quad \text{a.e. in } [0,1], \tag{36}$$

where the fundamental system $\Phi(t) \in \mathbb{R}^{(2n_x+n_\psi+n_y)\times(2n_x+n_\psi+n_y)}$ is the unique solution of

$$\Phi'(t) = B(t)\Phi(t), \qquad \Phi(0) = I. \tag{37}$$

(c) *The boundary value problem $T(\xi, y) = (\omega_1, \omega_2, \omega_3)^\top$ has a solution for every $(\omega_1, \omega_2, \omega_3)^\top$ and the inverse operator T^{-1} exists and it holds $\|T^{-1}\| \leq K$ for some constant K.*

Proof.

(a) Consider the equation $0 = G_d(0)\xi_0 - \omega_2(0)$. Since $M(0) = G_d(0) \cdot \hat{B}_2(0)$ is supposed to be non-singular, $G_d(0)$ has full row rank. Hence, there exists a QR decomposition

$$G_d(0)^\top = P \begin{pmatrix} R \\ 0 \end{pmatrix}, \qquad P = (\Pi_1, \Gamma) \in \mathbb{R}^{(2n_x+n_\psi+n_y)\times(2n_x+n_\psi+n_y)},$$

where $R \in \mathbb{R}^{n_y \times n_y}$ is nonsingular, P is orthogonal, $\Pi_1 \in \mathbb{R}^{(2n_x+n_\psi+n_y)\times n_y}$ is an orthonormal basis of $\mathrm{im}(G_d(0)^\top)$, $\Gamma \in \mathbb{R}^{(2n_x+n_\psi+n_y)\times(2n_x+n_\psi)}$ is a orthonormal basis of $\mathrm{im}(G_d(0)^\top)^\perp = \ker(G_d(0))$. Every $\xi_0 \in \mathbb{R}^{2n_x+n_\psi+n_y}$ can be expressed uniquely as $\xi_0 = \Pi_1 v + \Gamma\mu$ with $v \in \mathbb{R}^{n_y}$ and $\mu \in \mathbb{R}^{2n_x+n_\psi}$. Introducing this expression into the algebraic equation yields

$$0 = G_d(0)(\Pi_1 v + \Gamma\mu) - \omega_2(0) = R^\top v - \omega_2(0) \quad \Rightarrow \quad v = R^{-\top}\omega_2(0).$$

Hence, the consistent values are characterized by

$$\xi_0 = \Pi\omega_2(0) + \Gamma\mu, \qquad \Pi := \Pi_1 R^{-\top}.$$

(b) We differentiate the algebraic equation $0 = G_d(t)\xi(t) - \omega_2(t)$ and obtain

$$\begin{aligned} 0 &= G_d'(t)\xi(t) + G_d(t)\xi'(t) - \omega_2'(t) \\ &= \left(G_d'(t) + G_d(t)\hat{B}_d(t)\right)\xi(t) + G_d(t)\hat{B}_2(t)y(t) - \omega_2'(t) + G_d(t)\omega_1(t) \\ &= Q(t)\xi(t) + M(t)y(t) + q(t). \end{aligned}$$

We exploit the non-singularity of $M(t) = G_d(t) \cdot \hat{B}_2(t)$ in order to solve the equation w.r.t. y and obtain

$$y(t) = -M(t)^{-1}\left(q(t) + Q(t)\xi(t)\right).$$

Introducing this expression into the differential equation for ξ yields

$$\begin{aligned} \xi'(t) = \left(\hat{B}_d(t) - \hat{B}_2(t)M(t)^{-1}Q(t)\right)\xi(t) + \omega_1(t) - \hat{B}_2(t)M(t)^{-1}q(t) \\ = B(t)\xi(t) + \omega(t). \end{aligned}$$

Considering the representation of consistent initial values ξ_0 in (a) we are in the situation as in Hermes and Lasalle [16], p. 36, and the assertions follow likewise.

(c) Part (c) exploits the solution formulas in (a) and (b). Since

$$\|T^{-1}\| = \frac{1}{\inf\{\|T(\xi,y)\| \mid \|(\xi,y)\| = 1\}},$$

we must show that

$$\|(\omega_1,\omega_2,\omega_3)\|_{\Omega_1} \geq \frac{1}{K}\|(\xi,y)\|_{\Omega_0}$$

for all $(\omega_1,\omega_2,\omega_3) \in \Omega_1$ and $(\xi,y) \in \Omega_0$ solving the BVP

$$\begin{aligned} \xi'(t) - \hat{B}_d(t)\xi(t) - \hat{B}_2(t)y(t) &= \omega_1(t), \\ G_d(t)\xi(t) &= \omega_2(t), \\ E_0\xi(0) + E_1\xi(1) &= \omega_3. \end{aligned}$$

We note

$$\begin{aligned} \|Q\|_\infty &\leq \|G_d'\|_\infty + \|G_d\|_\infty\|\hat{B}_d\|_\infty \leq C + C^2 =: \kappa_1, \\ \|B\|_\infty &\leq \|\hat{B}_d\|_\infty + \|\hat{B}_2\|_\infty\|M^{-1}\|_\infty\|Q\|_\infty \leq C + CC_1\kappa_1 =: \kappa_2, \\ \|q\|_r &\leq \|\omega_2\|_{1,r} + \|G_d\|_\infty\|\omega_1\|_r \leq \max\{1,C\}\|(\omega_1,\omega_2,\omega_3)\|_{\Omega_1} \\ &=: \kappa_3\|(\omega_1,\omega_2,\omega_3)\|_{\Omega_1}, \\ \|\omega\|_r &\leq \|\omega_1\|_r + \|\hat{B}_2\|_\infty\|M^{-1}\|_\infty\|q\|_r \\ &\leq \|\omega_1\|_r + CC_1\|q\|_r \leq \max\{1, CC_1\kappa_3\}\|(\omega_1,\omega_2,\omega_3)\|_{\Omega_1} \\ &=: \kappa_4\|(\omega_1,\omega_2,\omega_3)\|_{\Omega_1}. \end{aligned}$$

The boundary condition is satisfied, if

$$\begin{aligned} \omega_3 &= E_0\xi(0) + E_1\xi(1) \\ &= E_0\left(\Pi\omega_2(0) + \Gamma\mu\right) + E_1\Phi(1)\left(\Pi\omega_2(0) + \Gamma\mu + \int_0^1 \Phi^{-1}(\tau)\omega(\tau)d\tau\right) \\ &= \left(E_0 + E_1\Phi(1)\right)\Gamma\mu + \left(E_0 + E_1\Phi(1)\right)\Pi\omega_2(0) \\ &\quad + E_1\Phi(1)\int_0^1 \Phi^{-1}(\tau)\omega(\tau)d\tau. \end{aligned}$$

Rearranging terms and exploiting $\Phi(0) = I$ yields

$$\begin{aligned} \left(E_0\Phi(0) + E_1\Phi(1)\right)\Gamma\mu = \omega_3 &- \left(E_0 + E_1\Phi(1)\right)\Pi\omega_2(0) \\ &- E_1\Phi(1)\int_0^1 \Phi^{-1}(\tau)\omega(\tau)d\tau. \end{aligned} \tag{38}$$

Consider the initial value problem

$$\tilde{\xi}'(t) = B(t)\tilde{\xi}(t) + \omega(t), \qquad \tilde{\xi}(0) = 0.$$

The solution is given by

$$\tilde{\xi}(t) = \int_0^t B(\tau)\tilde{\xi}(\tau) + \omega(\tau)d\tau = \Phi(t)\int_0^t \Phi^{-1}(\tau)\omega(\tau)d\tau.$$

Gronwall's lemma yields

$$\|\tilde{\xi}(t)\| \leq \|\omega\|_1 \exp(\|B\|_\infty) \leq \|\omega\|_1 \exp(\kappa_2).$$

Hölder's inequality implies

$$\|\tilde{\xi}(t)\| \leq \tilde{C}\|\omega\|_r \exp(\kappa_2) \leq \tilde{C}\kappa_4 \exp(\kappa_2)\|(\omega_1, \omega_2, \omega_3)\|_{\Omega_1}$$

for $1 \leq r \leq \infty$ and some constant $\tilde{C}$.
Similarly, we find

$$\|\xi(t)\| \leq \left(\|\Pi\omega_2(0) + \Gamma\mu\| + \tilde{C}\|\omega\|_r\right) \exp(\kappa_2).$$

For the fundamental system Φ we obtain

$$\|\Phi(t)\| \leq 1 + \|B\|_\infty \int_0^t \|\Phi(\tau)\| d\tau \leq \exp(\kappa_2).$$

Using the solution formula for ξ yields

$$\begin{aligned}
\xi(t) &= \Phi(t) \left(\Pi\omega_2(0) + \Gamma\mu + \int_0^t \Phi(\tau)^{-1}\omega(\tau) d\tau\right) \\
&= \Phi(t) \left(\Pi\omega_2(0) + \Gamma\mu\right) + \tilde{\xi}(t).
\end{aligned}$$

Equation (38) reads as

$$\left(E_0\Phi(0) + E_1\Phi(1)\right) \Gamma\mu = \omega_3 - \left(E_0 + E_1\Phi(1)\right) \Pi\omega_2(0) - E_1\tilde{\xi}(1).$$

Assumption (iii) and $\|\omega_2(0)\| \leq 2\tilde{C}\|\omega\|_{1,r}$ yields

$$\begin{aligned}
\kappa\|\mu\| &\leq \|\left(E_0\Phi(0) + E_1\Phi(1)\right) \Gamma\mu\| \\
&\leq \|\omega_3\| + 2\tilde{C}\left(\|E_0\| + \tilde{C}\|E_1\| \exp(\kappa_2)\right) \|\Pi\|\|\omega_2\|_{1,r} \\
&\qquad + \tilde{C}\|E_1\|\|\omega\|_r \exp(\kappa_2).
\end{aligned}$$

As the operators E_0, E_1 and Π are bounded, we find

$$\begin{aligned}
\|\mu\| \;&\leq\; \frac{1}{\kappa} \max\{1, 2\tilde{C}\left(\|E_0\| + \tilde{C}\|E_1\| \exp(\kappa_2)\right) \|\Pi\|, \\
&\qquad \tilde{C}\|E_1\|\kappa_4 \exp(\kappa_2)\}\|(\omega_1, \omega_2, \omega_3)\|_{\Omega_1} \\
&=: \kappa_5\|(\omega_1, \omega_2, \omega_3)\|_{\Omega_1}.
\end{aligned}$$

Moreover,

$$\begin{aligned}
\|\xi(t)\| \;&\leq\; \exp(\kappa_2) \max\{2\tilde{C}\|\Pi\|, \|\Gamma\|\kappa_5, \tilde{C}\kappa_4\}\|(\omega_1, \omega_2, \omega_3)\|_{\Omega_1} \\
&=: \kappa_6\|(\omega_1, \omega_2, \omega_3)\|_{\Omega_1}.
\end{aligned}$$

Minkowski's inequality yields

$$\|\xi'\|_r = \|B(\cdot)\xi(\cdot) + \omega(\cdot)\|_r \leq \|B(\cdot)\xi(\cdot)\|_r + \|\omega\|_r \leq \kappa_2\|\xi\|_r + \|\omega\|_r$$

and thus

$$\|\xi'\|_r \leq (\kappa_4 + \kappa_2\kappa_6)\|(\omega_1, \omega_2, \omega_3)\|_{\Omega_1}.$$

With $\kappa_7 := \max\{\kappa_6, \kappa_4 + \kappa_2\kappa_6\}$ we obtain $\|\xi\|_{1,r} \leq \kappa_7\|(\omega_1, \omega_2, \omega_3)\|_{\Omega_1}$.
Using formula (36) for y it follows $\|y\|_r \leq C_1 (\|q\|_r + \kappa_1\|\xi\|_r) \leq \kappa_8\|(\omega_1, \omega_2, \omega_3)\|_{\Omega_1}$ and $\kappa_8 := C_1(\kappa_3 + \kappa_1\kappa_6)$.
Finally the assertion follows because of

$$\|(\xi, y)\|_{\Omega_0} \leq \max\{\kappa_7, \kappa_8\}\|(\omega_1, \omega_2, \omega_3)\|_{\Omega_1} =: K\|(\omega_1, \omega_2, \omega_3)\|_{\Omega_1}.$$

Hence, in each iteration of Algorithm 1 we have to solve the linear boundary value problem given by the differential-algebraic equation (23) and the boundary condition (24). The differential-algebraic equation (23) has algebraic equations of index-1 and index-2.

Remark 2 Theorem 4 holds for every $1 \leq r \leq \infty$. In particular, this implies that every element $V \in \partial_* F(z)$ maps a function in Y_r to a function in Z_r. In particular, if $F(z^k) \in Y_\infty$ then $d^k = -V_k^{-1}F(z^k) \in Z_\infty$. $F(z^k) \in Y_\infty$ holds, if $z^k \in Z_\infty$. Hence, the smoothing operator S_k in step (3) of Algorithm 1 can be chosen to be the identity if the initial z^0 is chosen to be in Z_∞. Then the condition

$$\|S_k(z^k + d^k) - z_*\|_{Z_\infty} \leq C_S\|z^k + d^k - z_*\|_{Z_r}$$

reduces to

$$\|z^{k+1} - z_*\|_{Z_\infty} \leq C_S\|z^{k+1} - z_*\|_{Z_r}.$$

4 Globalization

One reason that makes the Fischer-Burmeister function appealing is the fact that its square

$$\phi(a, b) := \varphi(a, b)^2 = \left(\sqrt{a^2 + b^2} - a - b\right)^2$$

is continuously differentiable with $\phi'(a, b) = 2\varphi(a, b)v$, where $v \in \partial\varphi(a, b)$ is arbitrary. Hence, the mappings

$$(\bar{x}, \bar{y}, \bar{u}, \bar{\eta}) \in \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_c} \mapsto \phi(-c_i(\bar{x}, \bar{y}, \bar{u}), \bar{\eta}_i), \quad i = 1, \ldots, n_c$$

are continuously differentiable by the chain rule. This allows to globalize the local semi-smooth Newton's method using the squared L^2-norm of F as a merit function:

$$\begin{aligned}
\Theta(z) &:= \frac{1}{2}\|F(z)\|_{Y_2}^2 \\
&= \frac{1}{2}\int_0^1 \left(\|x'(t) - f(x(t), y(t), u(t))\|^2 + \|g(x(t))\|^2\right) dt \\
&\quad + \frac{1}{2}\int_0^1 \left(\left\|\lambda_f'(t) + H_x'[t]^\top\right\|^2 + \left\|H_y'[t]^\top\right\|^2 + \left\|H_u'[t]^\top\right\|^2\right) dt \\
&\quad + \frac{1}{2}\sum_{i=1}^{n_c}\int_0^1 \phi(-c_i(x(t), y(t), u(t)), \eta_i(t)) dt \\
&\quad + \frac{1}{2}\|\psi(x(0), x(1))\|^2 + \frac{1}{2}\|\lambda(0) + \psi_{x_0}'(x(0), x(1))^\top\sigma + g_x'(x(0))^\top\zeta\|^2 \\
&\quad + \frac{1}{2}\|\lambda(1) - \psi_{x_1}'(x(0), x(1))^\top\sigma\|^2.
\end{aligned}$$

Θ is Fréchet-differentiable in Z_∞ if f_0, f, g, c, ψ are twice continuously differentiable. An analysis of the derivative of Θ reveals that for d^k with $V_k(d^k) = -F(z^k)$ it holds

$$\Theta'(z^k)(d^k) = -2\Theta(z^k) = -\|F(z^k)\|_{Y_2}^2. \tag{39}$$

As a consequence, d^k is a direction of descent of Θ at z^k and the line-search in the following global version of the semi-smooth Newton's method is well-defined unless z^k is a zero of F.

Algorithm 2 (Global Semi-Smooth Newton's Method)

(0) Choose z^0, $\beta \in (0,1)$, $\sigma \in (0, 1/2)$.
(1) If some stopping criterion is satisfied, stop.
(2) Chose an arbitrary $V_k \in \partial_* F(z^k)$ and compute the search direction d^k from

$$V_k(d^k) = -F(z^k).$$

(3) Find smallest $i_k \in \mathbb{N}_0$ with

$$\Theta(z^k + \beta^{i_k} d^k) \leq \Theta(z^k) + \sigma\beta^{i_k}\Theta'(z^k)(d^k)$$

and set $\alpha_k = \beta^{i_k}$.
(4) Set $z^{k+1} = S_k(z^k + \alpha_k d^k)$, $k = k+1$, and goto (1).

Remark 3 According to the Remark 2 the smoothing operator S_k can be omitted.

The following global convergence result can be proven in the same way as Theorem 4.2 in Gerdts [13].

Theorem 5 *Let the inverse operators V_k^{-1} exist for all k and let $C > 0$ be a constant such that $\|V_k^{-1}\|_{\mathcal{L}(Y_\infty, Z_\infty)} \leq C$ holds for all k. Let z_* be an accumulation point of the sequence $\{z^k\}$ generated by the global semi-smooth Newton's method.*

Then, z_* is a zero of F.

Eventually the globalized semi-smooth Newton method accepts the step size $\alpha_k = 1$ and turns into the local method.

Theorem 6 *Let the assumptions of Theorems 1 and 5 be valid with $r = 2$.*

Then, for sufficiently large k the step length $\alpha_k = 1$ is accepted and the global method turns into the local one.

Proof The proof of the local convergence theorem 1 showed the superlinear convergence of the values $\|F(z^k)\|_{Y_r}$, i.e. for any $\varepsilon > 0$ there exists $\delta > 0$ such that for all $\|z - z_*\|_{Z_\infty} \le \delta$ it holds

$$\|z + d - z_*\|_{Z_\infty} \le \varepsilon \|z - z_*\|_{Z_\infty}, \qquad \|F(z + d)\|_{Y_r} \le \varepsilon \|F(z)\|_{Y_r},$$

where $d = -V^{-1}F(z)$, $V \in \partial_* F(z)$. In particular, with $z = z^k$ and $d = d^k$ there exists $\delta > 0$ such that for all $\|z^k - z_*\|_{Z_\infty} \le \delta$ it holds

$$\|z^k + d^k - z_*\|_{Z_\infty} \le \frac{1}{2}\|z^k - z_*\|_{Z_\infty}, \qquad \|F(z^k + d^k)\|_{Y_r} \le \sqrt{1 - 2\sigma}\|F(z^k)\|_{Y_r}.$$

With $r = 2$ this implies

$$\Theta(z^k + d^k) = \frac{1}{2}\|F(z^k + d^k)\|_{Y_2}^2 \le \frac{1 - 2\sigma}{2}\|F(z^k)\|_{Y_2}^2 = (1 - 2\sigma)\Theta(z^k)$$

resp.

$$\Theta(z^k + d^k) \le \Theta(z^k) - 2\sigma\Theta(z^k) = \Theta(z^k) + \sigma\Theta'(z^k)(d^k),$$

i.e. Armijo's line-search accepts $\alpha_k = 1$ and $z^{k+1} = z^k + d^k$. Furthermore, $\|z^{k+1} - z_*\|_{Z_\infty} \le \frac{1}{2}\|z^k - z_*\|_{Z_\infty} \le \delta$ and we are in the same situation as above and the argument could be repeated.

More advanced globalization strategies for inexact Newton methods or smoothing Newton methods can be found in a recent paper by Chen and Gerdts [3].

5 Computational Issues and Numerical Results

We give numerical results where the linear DAE boundary value problem (21)-(22) is solved using the symmetric collocation method of Kunkel and Stöver [21]. They use index reduction techniques in order to get a differentiation index of 1 and separation of differential and algebraic equations. Instead of numerical index reduction we will reduce the index likewise to the proof of theorem 4 (b), by replacing the index-2 constraint

$$g_x'(x^k(t))x(t) = -g(x^k(t))$$

by its time derivative

$$\frac{d}{dt}\left(g_x'\right)x + g_x'\dot{x} = -g_x'\dot{x}^k$$

resp.

$$\left(\frac{d}{dt}\left(g'_x\right)+g'_x f'_x\right)x+g'_x f'_y y+g'_x f'_u u=-g'_x f.$$

Consistency is preserved by adding the boundary condition

$$g'_x(x^k(0))x(0)=-g(x^k(0)).$$

It is not unusual that the linear operator V_k is singular due to contradicting or redundant boundary conditions and algebraic constraints. E.g. B_k in

$$\underbrace{\begin{pmatrix} g'_x & 0 \\ \psi'_{x_0} & \psi'_{x_1} \end{pmatrix}}_{B_k}\begin{pmatrix} x(0) \\ x(1) \end{pmatrix}=-\underbrace{\begin{pmatrix} g \\ \psi \end{pmatrix}}_{w(z^k)}. \tag{40}$$

might not have full row rank n_y+n_ψ for some intermediate iterate z^k. If this happens we propose the following modifications. First we determine a maximal index set I of linearly independent rows of B_k by QR-decomposition of $B_k^\top$. Let

$$i^* := \arg\max_{i\in I}|w_i(z^k)|$$

and let b_l denote the l-th row of B_k. Let us assume for a moment that $w_{i^*}(z^k)\neq 0$. Then we replace w by $\tilde{w}$ where

$$\tilde{w}_i(z):=\begin{cases} w_i(z), & \text{if } i\in I\setminus\{i^*\}, \\ w_{i^*}(z)+\sum_{j\in I^c}\frac{w_j(z^k)}{w_{i^*}(z^k)}w_j(z), & \text{if } i=i^*, \\ p_i(z), & \text{if } i\in I^c, \end{cases}$$

and $p(z):=(\zeta(0),\sigma(0))^\top$. In globalized semi-smooth Newton's method we now calculate the search direction from

$$\tilde{V}_k\tilde{d}^k=-\tilde{F}_k(z^k)$$

where $\tilde{V}_k$ is some element of $\partial_*\tilde{F}_k(z^k)$ and $\tilde{F}_k$ is F where the boundary conditions w in (40) are replaced by $\tilde{w}$. This means that the new boundary conditions read

$$b_i\tilde{x}_{01}=-w_i(z^k), \qquad \text{if } i\in I\setminus\{i^*\}, \tag{41}$$

$$b_{i^*}\tilde{x}_{01}+\sum_{j\in I^c}\frac{w_j(z^k)}{w_{i^*}(z^k)}b_j\tilde{x}_{01}=-w_{i^*}(z^k)-\sum_{j\in I^c}\frac{w_j(z^k)^2}{w_{i^*}(z^k)}, \qquad \text{if } i=i^*, \tag{42}$$

$$p_i(z)=-p_i(z^k), \qquad \text{if } i\in I^c, \tag{43}$$

where $\tilde{x}_{01}:=(\tilde{x}(0),\tilde{x}(1))^\top$. We motivate these modifications by showing that it still holds

$$\Theta'(z^k)(\tilde{d}^k)=-2\Theta(z^k). \tag{44}$$

Since almost all components of V_k and F remain unchanged, (44) reduces to

$$\begin{aligned}\Theta'(z^k)(\tilde{d}^k) + 2\Theta(z^k) &= \langle V_k\tilde{d}^k, F(z^k)\rangle_2 + \langle F(z^k), F(z^k)\rangle_2 \\ &= (B_k\tilde{x}_{01})^\top w(z^k) + w(z^k)^\top w(z^k) \\ &= w_{i^*}(z^k)b_{i^*}\tilde{x}_{01} + w_{i^*}(z^k)^2 \\ &\quad + \sum_{i\in I\setminus\{i^*\}} \left(w_i(z^k)b_i\tilde{x}_{01} + w_i(z^k)^2\right) \\ &\quad + \sum_{j\in I^c} \left(w_j(z^k)b_j\tilde{x}_{01} + w_j(z^k)^2\right).\end{aligned}$$

Introducing the expressions for $b_i\tilde{x}_{01}$ from (41) and $b_{i^*}\tilde{x}_{01}$ from (42) directly yields $\Theta'(z^k)(\tilde{d}^k) + 2\Theta(z^k) = 0$.

If $w_{i^*}(z^k) = 0$ or $I = \emptyset$ (e.g. $B_k = 0$) we set $\tilde{w}_i(z) := w_i(z)$ and $\tilde{w}_j(z) := p_j(z)$ for $i \in I$ and $j \in I^c$. Then we get

$$\Theta'(z^k)(\tilde{d}^k) = -2\Theta(z^k) + \sum_{j\in I^c} w_j(z^k)^2.$$

Since $2\Theta(z^k) = \|F(z^k)\|_{Y_2}^2 \geq w(z^k)^\top w(z^k)$, the search direction $\tilde{d}^k$ is at least a direction of descent.

Although the described modifications resolve a common situation in which V_k is singular, it is not guaranteed that $\tilde{V}_k$ is non-singular. In such a case one could try to find an alternative relaxation strategy, switch to gradient methods or restart with another initial guess. A globalization strategy which is able to handle singular operators V_k by switching to gradient steps is discussed in Chen and Gerdts [3].

The two following examples both have linearly dependent constraints (even at local minimizers) and we observe at least numerically that the method works well and we do not lose fast local convergence.

The following computations were performed on a shared memory 64-bit multiple core computer with 8 dual-core CPUs at 2.8 GHz processing speed. Symmetric collocation method yields a large and sparse linear system of equations which was solved in parallel using the software package PARDISO [27], [28]. The collocation method proposed in [21] works with two different interpolation schemes, a Gauß-scheme with q knots for the differential parts and a Lobatto-scheme with $q+1$ knots for the algebraic parts. For the following computations we split the overall time interval $[0, 1]$ in N_t equal sized subintervals.

Parameters in Armijo's line search rule are $\beta = 0.9$ and $\sigma = 0.1$. We observe that the number of iterations can be reduced significantly using a non-monotone line search rule.

5.1 2D-pendulum

The equations of motion in modeling of mechanical multi body systems are given by

$$\begin{aligned}\dot{q}(t) &= v(t),\\ M(q(t))\dot{v}(t) &= F(q(t),v(t),u(t)) - G'(q(t))^\top \nu(t),\\ 0_{n_G} &= G(q(t)),\end{aligned}$$

where q are generalized coordinates of the bodies, M is the symmetric and positive definite mass matrix, F combines generalized forces and $G = 0$ defines algebraic constraints. Multiplying the second equation with M^{-1} leads to a Hessenberg DAE which has differentiation index 3 if $\operatorname{rank}(G') = n_G$, see [12]. In this paper we discuss only index 2 DAEs. We reduce the index using the Gear-Gupta-Leimkuhler technique, see [8]:

$$\begin{aligned}\dot{q}(t) &= v(t) - G'(q(t))^\top \mu(t),\\ M(q(t))\dot{v}(t) &= F(q(t),v(t),u(t)) - G'(q(t))^\top \nu(t),\\ 0_{n_G} &= G(q(t)),\\ 0_{n_G} &= G'(q(t))v(t).\end{aligned}$$

With the notation from the previous sections we have $x := (q,v)^\top$, $y := (\nu,\mu)^\top$ and

$$\begin{aligned}f(x,y,u) &:= \begin{pmatrix} v - G'(q)^\top \mu \\ M(q)^{-1}\left(F(q,v,u) - G'(q)^\top \nu\right)\end{pmatrix},\\ g(x) &:= \begin{pmatrix} G(q) \\ G'(q)v \end{pmatrix}.\end{aligned}$$

The index is 2, since the matrix

$$g'_x(x)f'_y(x,y,u) = \begin{pmatrix} 0 & -G'(q)G'(q)^\top \\ -G'(q)M(q)^{-1}G'(q)^\top & -(G'(q)v)'_q G'(q)^\top \end{pmatrix}$$

is non-singular if $\operatorname{rank}(G'(q)) = n_G$.

We discuss the optimal control of a two dimensional pendulum. Let the pendulum be mounted in the origin, let $q := (x_1,x_2)^\top$ be the position of the mass and $v := (x_3,x_4)^\top$ its velocity. Let $M(q) := I_2$. The distance of the mass from the origin should remain constant which yields the algebraic constraint $G(q) := x_1^2 + x_2^2 - 1 = 0$. The pendulum can be controlled by the momentum u. We minimize the costs

$$\frac{1}{2}\int_0^T u(t)^2 dt$$

subject to the equations of motion

$$\begin{aligned}
\begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \end{pmatrix} &= \begin{pmatrix} x_3 \\ x_4 \end{pmatrix} - \begin{pmatrix} 2x_1y_2 \\ 2x_2y_2 \end{pmatrix}, \\
\begin{pmatrix} \dot{x}_3 \\ \dot{x}_4 \end{pmatrix} &= \begin{pmatrix} ux_2 \\ -a_g - ux_1 \end{pmatrix} - \begin{pmatrix} 2x_1y_1 \\ 2x_2y_1 \end{pmatrix}, \qquad a_g := 9.81\frac{m}{s^2}, \\
0 &= x_1^2 + x_2^2 - 1, \\
0 &= 2x_1x_3 + 2x_2x_4,
\end{aligned}$$

and we want to move the pendulum from the starting position $(1,0)$ and velocity $(0,0)$ to its equilibrium, e.g. the boundary conditions are given by

$$0 = \psi(x(0), x(T)) = (x_1(0) - 1, x_2(0), x_3(0), x_4(0), x_1(T), x_3(T))^\top .$$

Finally we restrict the control by box constraints

$$u_{\min} \leq u \leq u_{\max}.$$

The assumptions made for the local minimum principle in Section 2 are fulfilled with exception of the rank-assumption on

$$c(x(t), y(t), u(t)) := \begin{pmatrix} u_{\min} - u(t) \\ u(t) - u_{\max} \end{pmatrix}.$$

However, it can be shown, using a minimum principle with set constraints $u(t) \in \mathcal{U}$ that the necessary conditions also hold for box constraints. The operator

$$\mathcal{A} = \begin{pmatrix} 1 & -1 & 1 \\ s_1 & r_1 & 0 \\ -s_2 & 0 & r_2 \end{pmatrix}$$

is non-singular for any $(s_1, r_1) \in \partial\varphi(u^k(t) - u_{\min}, \eta_1^k)$, $(s_2, r_2) \in \partial\varphi(u_{\max} - u^k(t), \eta_2^k)$, due to Theorem 3. It holds $H''_{yu} \equiv 0$, $H''_{y\eta} \equiv 0$, $H''_{yy} \equiv 0$, $H''_{u\lambda_g} \equiv 0$ for all $z \in Z$ and therefore

$$F_1 = -g'_x f'_y, \quad G_d\hat{B}_2 = g'_x f'_y = \begin{pmatrix} 0 & -4x_1^2 - 4x_2^2 \\ -4x_1^2 - 4x_2^2 & -4x_1x_3 - 4x_2x_4 \end{pmatrix}.$$

$g'_x f'_y$ is non-singular and its inverse is bounded if $x_1^2 + x_2^2$ is bounded away from 0. This is fulfilled around a local minimizer x_*, since $x_{*,1}(t)^2 + x_{*,2}(t)^2 = 1$ for all $t \in [0, T]$, but it might be violated at some iterate x^k in a globalized method. In such a case one could restart the algorithm with different initial values or one could switch to gradient methods.

We give numerical results for parameters $T := 3$ and $-u_{\min} := u_{\max} := 2.7$. An initial guess was calculated by forward simulation of state and adjoint equation letting $x(t_0) := (1,0,0,0)^\top$, $\lambda_f(t_0) := (0,0,0,0)^\top$ and $u(t) = \eta_1(t) = \eta_2(t) = 0$. The numerical solution for $N_t = 1000$ and $q = 3$ is depicted in Figure 1 and the progress of the algorithm is shown in Table 1.

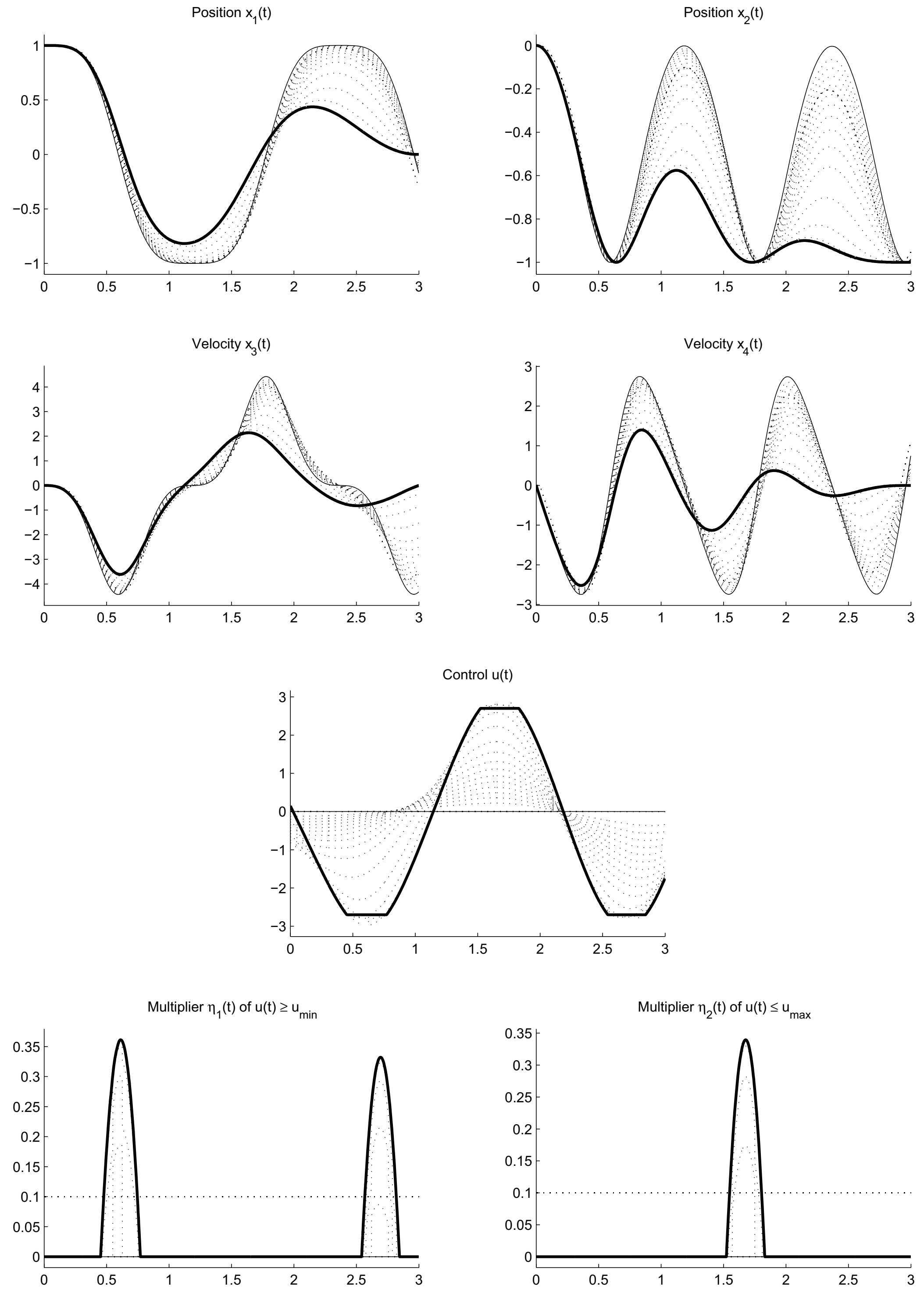

Fig. 1 Optimal control of the pendulum: converged solution (bold curves), initial guess (solid curve) and intermediate iterates (dashed curves)

Table 1 Optimal control of the pendulum: progress of semi-smooth Newton's method

k	$\int_0^1 f_0[t]dt$	α_{k-1}	$\|F(z^k)\|_2$
0	+0.000000000e+00		4.346837202e+00
1	+4.699355852e-02	0.05815	4.276531490e+00
2	+1.194251879e-01	0.03815	4.245650469e+00
3	+2.175784629e-01	0.03815	4.215799320e+00
4	+3.511018268e-01	0.04239	4.191093567e+00
5	+5.229507301e-01	0.04710	4.165010763e+00
6	+7.351681875e-01	0.05233	4.129532832e+00
7	+1.019076932e+00	0.06461	4.096028060e+00
8	+1.388198829e+00	0.07977	4.051127913e+00
9	+1.907341070e+00	0.10942	4.003788346e+00
10	+2.601024972e+00	0.15009	3.879776951e+00
11	+3.814497162e+00	0.28243	3.737060208e+00
12	+5.119627956e+00	0.43047	3.388155685e+00
13	+5.971125780e+00	0.59049	2.972992261e+00
14	+6.465774547e+00	1.00000	1.079417085e+00
15	+6.447073056e+00	1.00000	4.799579185e-02
16	+6.450874390e+00	1.00000	1.237672155e-02
17	+6.451931139e+00	1.00000	2.204752972e-03
18	+6.451987455e+00	1.00000	3.674825590e-04
19	+6.451989236e+00	1.00000	3.886533238e-05
20	+6.451989298e+00	1.00000	2.270141717e-06
21	+6.451989298e+00	1.00000	6.629377974e-08
22	+6.451989298e+00	1.00000	8.176486434e-11
23	+6.451989298e+00	1.00000	3.834227001e-14

5.2 2D-Navier-Stokes Problem

We illustrate the method on the distributed control of the two dimensional instationary incompressible Navier-Stokes equations on $Q := (0,T) \times \Omega$ with $\Omega = (0,1) \times (0,1)$. Please note that we don't claim that the presented discretization approach is the most efficient method for the Navier-Stokes equations. Our primary intention is to create a large-scale DAE optimal control problem which allows to test the performance of the semi-smooth Newton method.

The task is to minimize the distance to the desired velocity field

$$\begin{aligned} y_d(t,x_1,x_2) &= (-q(t,x_1)q'_{x_2}(t,x_2), q(t,x_2)q'_{x_1}(t,x_1))^\top, \\ q(t,z) &= (1-z)^2(1-\cos(2\pi z t)) \end{aligned}$$

within a given time $T > 0$.

Minimize

$$\frac{1}{2}\int_Q \|y(t,x_1,x_2) - y_d(t,x_1,x_2)\|^2 dx_1 dx_2 dt + \frac{\delta}{2}\int_Q \|u(t,x_1,x_2)\|^2 dx_1 dx_2 dt \tag{45}$$

subject to

$$
\begin{aligned}
y_t &= \tfrac{1}{Re}\Delta y - (y \cdot \nabla)y - \nabla p + u, \\
0 &= \operatorname{div}(y), \\
y(0, x_1, x_2) &= 0, \qquad (x_1, x_2) \in \Omega, \\
y(t, x_1, x_2) &= 0, \qquad (t, x_1, x_2) \in (0, T) \times \partial\Omega,
\end{aligned}
\tag{46}
$$

and the control constraints

$$u_{min} \leq u \leq u_{max}.$$

$y = (v, w)^\top$ denotes the velocity vector and p the pressure. The instationary incompressible Navier-Stokes equations can be viewed as a partial differential-algebraic equation.

We discretize the problem in space on an equally spaced mesh with step-length $h = \frac{1}{N}$, $N \in \mathbb{N}$, while the time stays continuous. This refers to the method of lines. Let $y_{ij}(t) = (v_{ij}(t), w_{ij}(t))^\top \approx y(t, x_{1,i}, x_{2,j}), p_{ij}(t) \approx p(t, x_{1,i}, x_{2,j})$ and $u_{ij}(t) \approx u(t, x_{1,i}, x_{2,j})$, $i, j = 0, \ldots, N$ denote the approximations at the grid points. Using these definitions finite differences discretization scheme reads

$$
\begin{aligned}
\Delta y|_{(t,x_{1,i},x_{2,j})} &\approx \frac{1}{h^2}\big(y_{i+1,j}(t) + y_{i-1,j}(t) + y_{i,j+1}(t) + y_{i,j-1}(t) \\
&\qquad -4y_{i,j}(t)\big), \\
(y \cdot \nabla)y|_{(t,x_{1,i},x_{2,j})} &\approx \frac{1}{2h}\big(v_{ij}(t)\left(y_{i+1,j}(t) - y_{i-1,j}(t)\right) \\
&\qquad + w_{ij}(t)\left(y_{i,j+1}(t) - y_{i,j-1}(t)\right)\big), \\
\nabla p|_{(t,x_{1,i},x_{2,j})} &\approx \frac{1}{h}\big(p_{i+1,j}(t) - p_{i,j}(t), p_{i,j+1}(t) - p_{i,j}(t)\big)^\top, \\
\operatorname{div}(y)|_{(t,x_{1,i},x_{2,j})} &\approx \frac{1}{h}\big(v_{i,j}(t) - v_{i-1,j}(t) + w_{i,j}(t) - w_{i,j-1}(t)\big),
\end{aligned}
$$

for $i, j = 1, \ldots, N-1$. The undefined pressure components $p_{i,j}$ with $i = N$ or $j = N$ are set to zero.

Introducing these approximations into the optimal control problem and exploiting the boundary conditions $y_{i,0}(t) = y_{i,N}(t) = 0$ for $i = 1, \ldots, N-1$ and $y_{0,j}(t) = y_{N,j}(t) = 0$ for $j = 1, \ldots, N-1$ yields a DAE optimal control problem with a differential-algebraic equation of index two:

Minimize

$$\frac{1}{2}\int_0^T \|y_h(t) - y_{d,h}(t)\|^2 dt + \frac{\delta}{2}\int_0^T \|u_h(t)\|^2 dt \tag{47}$$

subject to the DAE

$$
\begin{aligned}
y_h'(t) &= \frac{1}{Re}A_h y_h(t) - \frac{1}{2}\begin{pmatrix} y_h(t)^\top Q_{h,1} y_h(t) \\ \vdots \\ y_h(t)^\top Q_{h,2(N-1)^2} y_h(t) \end{pmatrix} - B_h p_h(t) + u_h(t), \\
0 &= B_h^\top y_h(t),
\end{aligned}
\tag{48}
$$

the initial values

$$y_h(0) = 0,$$

and the control constraints

$$u_{min} \leq u_h(t) \leq u_{max}.$$

Herein,

$$\begin{aligned} y_h &= (y_{1,1}, \ldots, y_{N-1,1}, y_{1,2}, \ldots, y_{N-1,2}, \ldots, y_{1,N-1}, \ldots, y_{N-1,N-1})^\top, \\ p_h &= (p_{1,1}, \ldots, p_{N-1,1}, p_{1,2}, \ldots, p_{N-1,2}, \ldots, p_{1,N-1}, \ldots, p_{N-1,N-1})^\top, \\ u_h &= (u_{1,1}, \ldots, u_{N-1,1}, u_{1,2}, \ldots, u_{N-1,2}, \ldots, u_{1,N-1}, \ldots, u_{N-1,N-1})^\top. \end{aligned}$$

The matrices $A_h \in \mathbb{R}^{2(N-1)^2 \times 2(N-1)^2}$ and $B_h \in \mathbb{R}^{2(N-1)^2 \times (N-1)^2}$ represent the discretized Laplacian resp. the discretized gradient. $Q_{h,i} \in \mathbb{R}^{2(N-1)^2 \times 2(N-1)^2}$ is the Hessian of the i-th component of the discretized convective term w.r.t. y_h, e.g.

$$\begin{aligned} q_{ij}(t) &= (y \cdot \nabla) y|_{(t,x_{1,i},x_{2,j})} \in \mathbb{R}^2, \\ Q_{h,2(i+j(N-1))-1} &= \nabla^2_{y_h} q_{ij,1}(t), \quad i,j = 1,\ldots,N-1, \\ Q_{h,2(i+j(N-1))} &= \nabla^2_{y_h} q_{ij,2}(t), \quad i,j = 1,\ldots,N-1. \end{aligned}$$

Note that $Q_{h,i}$ does not depend on $y_h(t)$, since the convective term is quadratic.

We give results for parameters $T = 2$, $\delta = 5 \cdot 10^{-6}$, $Re = 1$, $-u_{min} = u_{max} = 200$ and $N = 36$, $N_t = 60$, $q = 2$. Then the DAE optimal control problem has $n_x = 2(N-1)^2 = 2450$ differential variables, $n_y = (N-1)^2 = 1225$ algebraic variables and $n_u = 2450$ controls. The linear system which has to be solved in each iteration has 2649675 equations.

As initial guess we take the solution of the unconstrained Stokes problem (e.g. $Re = 1$, $Q_{h,i} = 0$ for $i = 1, \ldots, n_x$, $u_{min} = -\infty$, $u_{max} = \infty$) and set $\eta = 0$. Solution of the unconstrained Stokes problem only needs one iteration, since F is linear.

The desired flow, controlled flow and the control are depicted in Figure 2. An animation of the flow can be downloaded from the webpage of the first author (http://web.mat.bham.ac.uk/M.Gerdts/movies.htm). The regular structure of the control at $t = 1.3$ and $t = 1.966$ results from the constraints which are active in the lower left quarter. The progress of the algorithm is shown in Table 2.

References

1. A. Backes, *Extremalbedingungen für Optimierungs-Probleme mit Algebro-Differentialgleichungen*, PhD thesis, Mathematisch-Naturwissenschaftliche Fakultät, Humboldt-Universität Berlin, Berlin, Germany, 2006.
2. K. E. Brenan, S. L. Campbell, and L. R. Petzold, *Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations*, vol. 14 of Classics In Applied Mathematics, SIAM, Philadelphia, 1996.

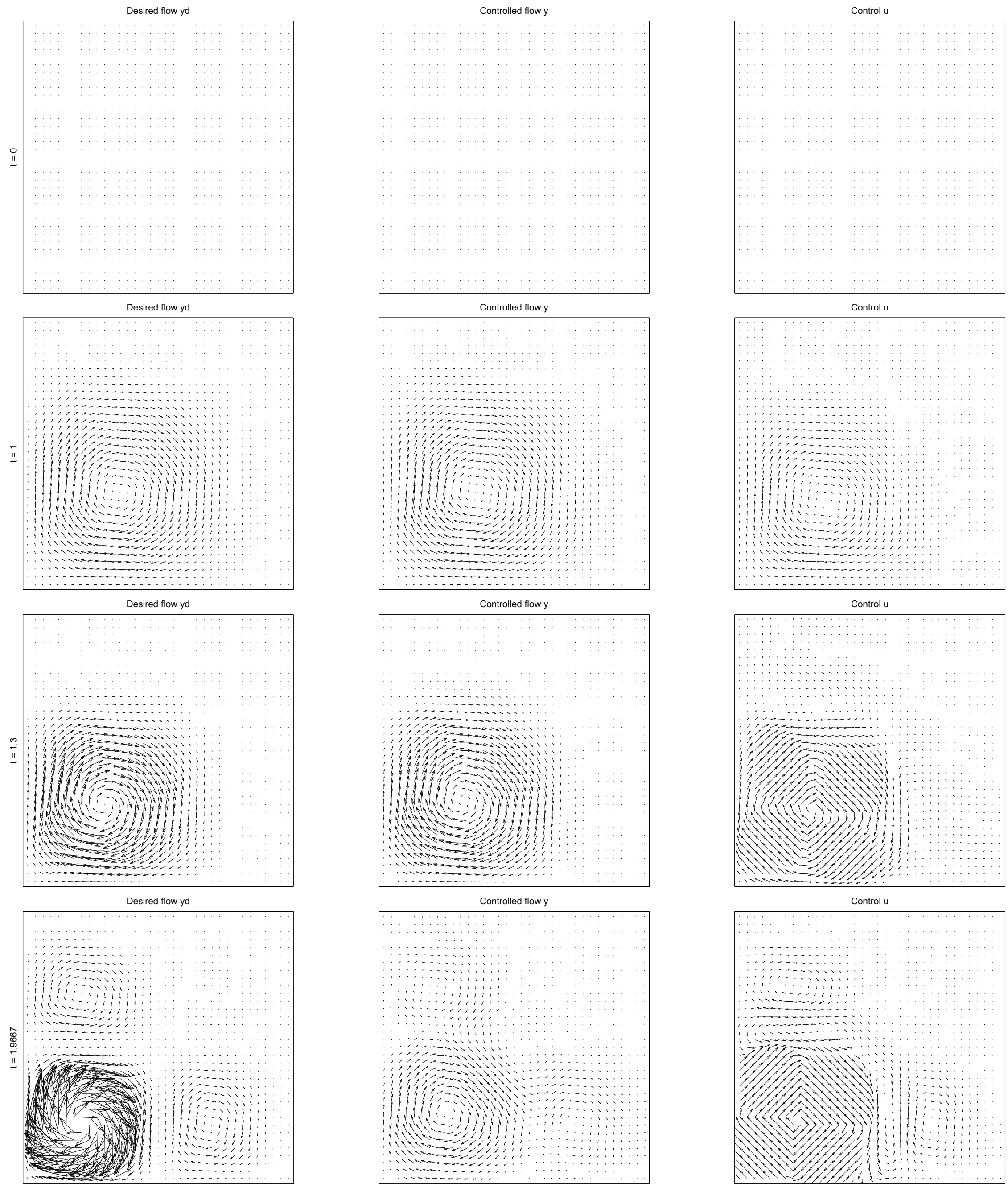

Fig. 2 Optimal control of Navier-Stokes equations. Desired flow (left), controlled flow (middle) and control (right) at $t = 0$, $t = 1.0$, $t = 1.3$ and $t = 1.966$.

3. J. Chen and M. Gerdts, *Numerical solution of control-state constrained optimal control problems with inexact nonsmooth and smoothing newton methods*, submitted, (2008).
4. X. Chen, Z. Nashed, and L. Qi, *Smoothing methods and semismooth methods for nondifferentiable operator equations*, SIAM Journal on Numerical Analysis, 38 (2000), pp. 1200–1216.
5. F. H. Clarke, *Optimization and Nonsmooth Analysis*, John Wiley & Sons, New York, 1983.
6. A. Fischer, *A special Newton-type optimization method*, Optimization, 24 (1992), pp. 269–284.

Table 2 Optimal control of Navier-Stokes equations: progress of semi-smooth Newton's method, line search was done by a non-monotone Armijo's rule

k	$\int_0^1 f_0[t]dt$	α_{k-1}	$\|F(z^k)\|_2$
0	+3.277938099e+02		3.305900577e+04
1	+8.654731485e+02	1.00000	1.577364410e+04
2	+9.326826159e+02	1.00000	2.100321310e+03
3	+9.364289058e+02	1.00000	2.639650877e+02
4	+9.364430997e+02	1.00000	5.551137024e+00
5	+9.349821987e+02	1.00000	5.270667106e+02
6	+9.342838408e+02	1.00000	1.663214177e+01
7	+9.342476168e+02	1.00000	1.192784778e+01
8	+9.342477269e+02	1.00000	4.781006076e-02
9	+9.342328733e+02	1.00000	8.525426187e-02
10	+9.342288904e+02	1.00000	5.372400865e-01
11	+9.342286947e+02	1.00000	2.789217897e-01
12	+9.342287084e+02	1.00000	1.739583457e-05
13	+9.342287063e+02	1.00000	5.764140637e-06
14	+9.342287069e+02	1.00000	5.549459285e-07
15	+9.342287078e+02	1.00000	1.526578112e-07
16	+9.342287078e+02	1.00000	1.211640685e-09

7. ———, *Solution of monotone complementarity problems with locally Lipschitzian functions*, Mathematical Programming, 76 (1997), pp. 513–532.
8. C. W. Gear, B. Leimkuhler, and G. K. Gupta, *Automatic integration of Euler-Lagrange equations with constraints*, Journal of Computational and Applied Mathematics, 12/13 (1985), pp. 77–90.
9. M. Gerdts, *Local minimum principle for optimal control problems subject to index-two differential-algebraic equations*, Journal of Optimization Theory and Applications, 130 (2006), pp. 443–462.
10. ———, *Representation of the Lagrange multipliers for optimal control problems subject to differential-algebraic equations of index two*, Journal of Optimization Theory and Applications, 130 (2006), pp. 231-251.
11. ———, *Direct Shooting Method for the Numerical Solution of Higher Index DAE Optimal Control Problems*, Journal of Optimization Theory and Applications, 117 (2003), pp. 267–294.
12. ———, *Optimal control and real-time optimization of mechanical multi-body systems*, ZAMM, 83 (2003), pp. 705–719.
13. ———, *Global convergence of a nonsmooth Newton method for control-state constrained optimal control problems*, SIAM Journal on Optimization, 19 (2008), pp. 326–350.
14. D. M. Gritsis, C. C. Pantelides, and R. W. H. Sargent, *Optimal control of systems described by index two differential-algebraic equations*, SIAM Journal on Scientific Computing, 16 (1995), pp. 1349–1366.
15. E. Hairer and G. Wanner, *Solving ordinary differential equations II: Stiff and differential-algebraic problems*, vol. 14, Springer Series in Computational Mathematics, Berlin-Heidelberg-New York, 2 ed., 1996.
16. H. Hermes and J. P. Lasalle, *Functional Analysis and Time Optimal Control*, vol. 56 of Mathematics in Science and Engineering, Academic Press, New York, 1969.
17. H. Jiang, *Global convergence analysis of the generalized Newton and Gauss-Newton methods of the Fischer-Burmeister equation for the complementarity problem*, Mathematics of Operations Research, 24 (1999), pp. 529–543.
18. B. Kummer, *Newton's method for non-differentiable functions*, in Advances in Mathematical Optimization, J. Guddat et al., ed., Berlin, 1988, Akademie-Verlag, pp. 171–194.

19. ———, *Newton's method based on generalized derivatives for nonsmooth functions: convergence analysis*, in Advances in Optimization, W. Oettli and D. Pallaschke, eds., Berlin, 1991, Springer, pp. 171–194.
20. P. Kunkel and V. Mehrmann, *Differential-algebraic equations. Analysis and numerical solution*, European Mathematical Society Publishing House, Zurich, 2006.
21. P. Kunkel and R. Stöver, *Symmetric collocation methods for linear differential-algebraic boundary value problems.*, Numer. Math., 91 (2002), pp. 475–501.
22. C. C. Pantelides, R. W. H. Sargent, and V. S. Vassiliadis, *Optimal Control of Multistage Systems Described by High-Index Differential-Algebraic Equations*, in Computational Optimal Control, R. Bulirsch, ed., vol. 115 of International Series of Numerical Mathematics, Basel, 1994, Birkhäuser, pp. 177–191.
23. L. R. Petzold, *Differential/algebraic equations are not ODE's*, SIAM Journal on Scientific and Statistical Computing, 3 (1982), pp. 367–384.
24. L. Qi, *Convergence analysis of some algorithms for solving nonsmooth equations*, Mathematics of Operations Research, 18 (1993), pp. 227–244.
25. L. Qi and J. Sun, *A nonsmooth version of Newton's method*, Mathematical Programming, 58 (1993), pp. 353–367.
26. T. Roubicek and M. Valásek, *Optimal control of causal differential-algebraic systems*, Journal of Mathematical Analysis and Applications, 269 (2002), pp. 616–641.
27. O. Schenk and K. Gärtner, *Solving Unsymmetric Sparse Systems of Linear Equations with PARDISO.*, Journal of Future Generation Computer Systems, 20 (2002), pp. 475–487.
28. ———, *On fast factorization pivoting methods for sparse symmetric indefinite systems.*, ETNA, Electron. Trans. Numer. Anal., 23 (2006), pp. 158–179.
29. V. H. Schulz, H. G. Bock, and M. C. Steinbach, *Exploiting invariants in the numerical solution of multipoint boundary value problems for DAE*, SIAM Journal on Scientific Computing, 19 (1998), pp. 440–467.
30. M. Ulbrich, *Nonsmooth Newton-like Methods for Variational Inequalities and Constrained Optimization Problems in Function Spaces*, Habilitation, Technical University of Munich, Munich, 2002.
31. ———, *Semismooth newton methods for operator equations in function spaces*, SIAM Journal on Optimization, 13 (2003), pp. 805–841.