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A multipoint shooting feasible-SQP method for optimal control of state-constrained parabolic DAE systems

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***Abstract*—Optimal control problem for parabolic differential-algebraic equations (PDAE) systems with spatially sensitive state-constraints and technological constraints is considered. Multipoint shooting approach is proposed to attack such problems. It is well suited to deal with unstable and ill-conditioned PDAE systems. This approach consists in the partitioning of the time-space domain into shorter layers, which allows us to fully parallelize the computations and to employ the reliable PDAE solvers. A new modified method of this kind is developed. It converts the multipoint shooting problem having mixed equality and inequality constraints into the purely inequality constrained problem. The results of the consecutive layer shots are exploited to determine a feasible shooting solution of the converted problem. The knowledge of such a solution is crucial for the use of highly efficient feasible-SQP methods avoiding the incompatibility of the constraints of the QP subproblems (versus the infeasible path SQP methods). The applications of the method proposed to the optimization of some heat transfer processes as well as chemical production processes performed in tubular reactors are discussed.**

I. Introduction

ADVANCED technological processes are often performed in distributed-parameter systems. A wide class of such processes is described by parabolic differential-algebraic equations including heat transfer processes and chemical production processes performed in tubular or multizone reactors [3],[9],[11],[2]. Many of them exhibit unstable modes and high sensitivity to parameter changes. In a consequence we can deal with unbounded state profiles and ill-conditioned optimization problems if the single shooting method is applied to optimize the system performance [2]. The multipoint shooting approach, known from the modelling of lumped parameter systems [10], can also be useful for distributed parameter systems to resolve the difficulties with their unstable and highly sensitive modes [5],[6],[13]. Moreover, it ensures the full parallelization of the computations necessary to employ advanced superlinearly convergent optimization methods such as the sequential quadratic programming (SQP) method or the interior point (IP) method [1]. However, the main elaborations on this subject deal with infeasible path approach, where all the constraints of the optimization problem may be violated on the current iteration. This may lead to the incompatibility of the constraints of the QP subproblems, which complicates the SQP algorithm. Its regularization may be required with the use, for example, the homotopy approach [2].

In the present paper the feasible-SQP method, known in many variants as the nonlinear programming methods [4],[7],[15], is developed as a method specialized in the multipoint shooting approach to the optimal control of PDAE systems. The exploitation of the specific structure of the method proposed enables us to resolve the difficult problem of obtaining of a feasible initial solution guaranteeing the compatibility of QP subproblems exploited in the process optimization.

Notation: $L_\infty(\Omega, R^n), W_\infty^{\alpha,\beta}(\Omega, R^n)$, and $PC(\Omega, R^n)$ the spaces of n-dimensional essentially bounded, essentially bounded derivatives and piecewise continuous functions defined on Ω, and $S_r([t_0, t_f], R^n)$ the space of n-dimensional r-step functions defined on the interval $[t_0, t_f]$.

II. Optimal control problem for parabolic DAE systems

Consider the following optimal control for parabolic DAE systems (the PD problem): minimize the objective function

$$\mathcal{J}(x, z, u, u_0, p) \doteq \int_0^\tau \int_0^1 h_0(x(t,s), z(t,s), u(t,s), p)dtds + \int_0^\tau h_1(x(t,1), z(t,1), u_0(t), p)dt \quad (1)$$

subject to a system of parabolic differential-algebraic equations (PDAE) of index one

$$x_t(t,s) = f(x(t,s), z(t,s), x_s(t,s), x_{ss}(t,s), u(t,s), p), \quad (2)$$

$$0 = g(x(t,s), z(t,s), u(t,s), p), \quad (t,s) \in \Omega_\tau, \quad (3)$$

to the boundary conditions

$$b_i(x(t,i), z(t,i), u_0(t), p) = 0, \quad t \in I_\tau \quad (i = 0, 1), \quad (4)$$

to the technological constraint

$$\int_0^\tau h(x(t,1), z(t,1), p)dt = 0, \quad (5)$$

to the box constraints

$$x(t,s) \in X(s),\ z(t,s) \in Z(s),\ u(t,s) \in U,\ (t,s) \in \Omega_\tau,$$
$$(t,s) \in \Omega_\tau,\ \ u_0(t) \in U_0,\ \ t \in I_\tau,\ \ p \in P, \quad (6)$$

and to the physical realizability conditions for the distributed and boundary control

$$u \in PC(\Omega_\tau, R^{n_u}),\ \ u_0 \in PC(I_\tau, R^{n_v}), \quad (7)$$

where $I_\tau \doteq [0,\tau]$ is the time horizon, $\Omega_\tau \doteq I_\tau \times I$ is the time-space domain, $x \in W_\infty^{1;2}(\Omega_\tau, R^{n_x})$ is the differential state trajectory of the PDAE system, $z \in L_\infty(\Omega_\tau, R^{n_z})$ is its algebraic state trajectory, $u \in L_\infty(\Omega_\tau, R^{n_u})$ is its distributed control, , $u_0 \in L_\infty(I_\tau, R^{n_{u_0}})$ is its boundary control, $p \in R^p$ is its global parameter, and $X(s) \doteq [x_-(s), x_+(s)]$, $Z(s) \doteq [z_-(s), z_+(s)]$, $U \doteq [u_-, u_+]$, $U_0 \doteq [u_{0-}, u_{0+}]$,, and $P \doteq [p_-, p_+]$ are boxes with the spatially sensitive bounds $x_\pm(s) \in R^{n_x}$, $z_\pm(s) \in R^{n_z}$, $u_\pm \in R^{n_p}$, $u_{0\pm} \in R^{n_{u_0}}$ and $p_\pm \in R^{n_p}$, and the functions

$$h_i : R^{n_x} \times R^{n_z} \times R^{n_{u^i}} \times R^{n_p} \to R\ \ (i = 0,1\ \ u^0 \doteq u, u^1 \doteq u_0),$$
$$h : R^{n_x} \times R^{n_z} \times R^{n_p} \to R^{n_h},$$
$$f : R^{n_x} \times R^{n_z} \times R^{n_u} \times R^p \to R^{n_x},$$
$$g : R^{n_x} \times R^{n_z} \times R^{n_u} \times R^p \to R^{n_z},$$
$$b_i : R^{n_x} \times R^{n_z} \times R^{n_{u_0}} \times R^{n_p} \to R^{n_{b_i}}\ \ \ (i = 0,1)$$

are twice continuously differentiable in all their arguments, while $X(s)$ and $Z(s)$ are bounded point to set mappings.

We use the time scaling $t := t/\tau$ to normalize the time horizon to the unit interval $t \in I$, and to include the variable process duration τ to the global parameter p, which may also encompass the technological and design variables (such as the level of the fixed bed catalyst or the reactor volume in chemical production processes), and the slack variables converting the technological inequality constraints into the equality ones. We reduce the general control and state inequality path constraints $q(x(t,s), z(t,s), u(t,s), p) \le 0$ into the equality form (3) by means of the slack control $\tilde{u}(t,s)$ fulfilling the condition $q(x(t,s), z(t,s), u(t,s), p) + \tilde{u}(t,s) = 0$. Thus the formulation (1)-(7) encompasses a wide class of optimal control problems for PDAE systems with the boundary and distributed controls.

III. Time-space multipoint shooting feasible-SQP method

We discretize the time coordinate $t_k = k/l\ \ (k = 0,1,...,l)$ and the space coordinate $s_i = i/j\ \ \ (i = 0,1,...,j)$. We connect with the time-space layer $[t_k, t_{k+1}] \times [s_i, s_{i+1}]$ $(i = 0,1,...,j)$ its shooting differential states $x_{ik} \in R^{n_x}$, its shooting algebraic states $z_{ik} \in R^{n_z}$, its shooting control variables $u_{ik} \doteq (u_{ik1}^T, u_{ik2}^T, ..., u_{ikr_{ik}}^T)^T \in R^{n_{u_{ik}}}$ $(n_{u_{ik}} \doteq n_u r_{ik},\ r_{il} \doteq 0,\ u_{il1} \doteq u_{i,l-1,r_{i,l-1}})$, its shooting global parameters $p_{ik} \in R^{n_p}$, its shooting optimization variables $w_{ik} \doteq (x_{ik}^T, z_{ik}^T, u_{ik}^T, p_{ik}^T)^T \in R^{n_{w_{ik}}}$ $(n_{w_{ik}} \doteq n_x + n_z + n_{u_{ik}} + n_p)$, its layer shooting optimization variable $w_k \doteq (w_{0k}^T, w_{1k}^T, ..., w_{jk}^T)^T \in R^{n_{w_k}}$ $(n_{w_k} \doteq \sum_{i=0}^j n_{w_{ik}})$, its differential state trajectories $\widetilde{x}_{ik} \in W_\infty^1([t_k, t_{k+1}], R^{n_x})$ determined by w_k, its algebraic state trajectories $\widetilde{z}_{ik} \in L_\infty([t_k, t_{k+1}], R^{n_x})$ determined by w_k, and its controls $\widetilde{u}_{ik} \in S_{r_{ik}}([t_k, t_{k+1}], R^{n_u})$ determined by u_{ik}. We include the boundary control shooting variables into the control variable u_{0k}, i.e. $u_{0k} \doteq (u_{0k1}^T, u_{0k2}^T, ..., u_{0kr_k}^T, u_{0k,r_k+1}^T, ..., u_{0kr_{0k}}^T)^T$, where $u_{0kr} \in R^{n_{u_0}}$ $(r = 1,2,...,r_k)$ are the coefficient of the boundary control, while $u_{0kr} \in R^{n_u}$ $(r = r_k+1, r_k+2, ..., r_{ik})$ are the coefficients of the distributed control variable connected with the 0th spatial element. We reformulate the problem discussed as the multipoint shooting PDAE optimal control problem (the MSPD problem): minimize the objective function

$$J(w) \doteq \sum_{i=0}^{j-1}\sum_{k=0}^{l-1} \delta_j \int_{t_k}^{t_{k+1}} h_0(\widetilde{x}_{ik}(t), \widetilde{z}_{ik}(t), \widetilde{u}_{ik}(t), p_{ik})$$
$$+ \sum_{k=0}^{l-1} \int_{t_k}^{t_{k+1}} h_1(\widetilde{x}_{jk}(t), \widetilde{z}_{jk}(t), \widetilde{u}_{0k}(t), p_{jk}) \quad (8)$$

subject to the continuity conditions for the differential state trajectory and the shooting parameters

$$\widetilde{x}_{ik}(t_{k+1}) = x_{i,k+1},\ \ p_{ik} = p_{i,k+1}\ \ (i = 0,1,...,j;$$
$$k = 0,1,...,l-1), \quad (9)$$

to the consistency equations for the algebraic states and the boundary conditions

$$g_{ik}(x_{ik}, z_{ik}, u_{ik}, p_{ik}) = 0\ \ (i = 0,1,...,j;\ k = 0,1,...,l), \quad (10)$$

to the technological constraint

$$\sum_{k=0}^{l-1} \int_{t_k}^{t_{k+1}} h(\widetilde{x}_{jk}(t), \widetilde{z}_{jk}(t), \widetilde{u}_{0k}(t), p_{jk}) = 0, \quad (11)$$

and to the bound constraints

$$x_{ik} \in X_i,\ \ z_{ik} \in Z_i,\ \ u_{ik} \in U_{ik},\ \ p_{ik} \in P$$
$$(i = 0,1,...,j;\ k = 0,1,...,l), \quad (12)$$

where $\delta_j \doteq 1/j$, and the boundary conditions are incorporated into the consistency equations

$$g_{ik}(x_{ik}, z_{ik}, u_{ik}, p_{ik}) \doteq$$
$$(\tilde{g}^T(x_{0k}, z_{0k}, u_{0k}, p_{0k}), \tilde{b}_0^T(x_{0k}, z_{0k}, u_{0k}, p_{0k})))^T\ \ (i = 0),$$

and

$$g_{ik}(x_{ik}, z_{ik}, u_{ik}, p_{ik}) \doteq g(x_{ik}, z_{ik}, u_{ik}, p_{ik})\ \ (0 < i < j),$$

and

$$g_{ik}(x_{ik}, z_{ik}, u_{ik}, p_{ik}) \doteq$$
$$(g^T(x_{jk}, z_{jk}, u_{jk}, p_{jk}), \tilde{b}_1^T(x_{jk}, z_{jk}, u_{0k}, p_{jk})))^T\ \ (i = j),$$

and $w \doteq (w_0^T, w_1^T, ..., w_l^T)^T \in R^{n_w}$ $(n_w \doteq \sum_{k=0}^{l} n_{w_k})$ is the shooting optimization variable, and $X_i \doteq [x_{i-}, x_{i+}]$, $x_{i\pm} \doteq x_\pm(s_i)$, $Z_i \doteq [z_{i-}, z_{i+}]$, $z_{i\pm} \doteq z_\pm(s_i)$, $U_{ik} \doteq [u_{ik-}, u_{ik+}]$, $u_{ik\pm} \doteq (\underbrace{u_\pm^T, u_\pm^T, ..., u_\pm^T}_{r_{ik}+1\ times})^T$, and $\tilde{b}_i$ $(i = 0, 1)$ are the modifications of the functions b_i connected with the redefinition of the controls u_{0k}.

Let $X_{i\varepsilon_i} \doteq [\varepsilon_i + x_{i-}, -\varepsilon_i + x_{i+}]$ $(\varepsilon_i \in R_+^{n_x})$ and $Z_{i\epsilon_i} \doteq [\epsilon_i + z_{i-}, -\epsilon_i + z_{i+}]$ $(\epsilon_i \in R_+^{n_z})$ be the restricted box sets for the differential and algebraic states, and let

$$\varepsilon_{in}, \epsilon_{in}, \widetilde{x}_{ikn}, x_{ikn}, p_{ikn}, x_{in-}, x_{in+}, z_{in-}, z_{in+}, g_{ikn}, h_n$$

be the nth coordinates of the quantities

$$\varepsilon_i, \epsilon_i, \widetilde{x}_{ik}, x_{ik}, p_{ik}, x_{i-}, x_{i+}, z_{i-}, z_{i+}, g_{ik}, h.$$

Algorithm 1: The conversion of the time-space shooting problem (8)-(12) for the PDAE system (the MSPD problem) to the parametric MSPD problem (the MSPD$_c$ problem) with a known feasible initial solution.

Step 0: Choose $\varepsilon_i = 0.05(x_{i+} - x_{i-})$, $\epsilon_i = 0.05(z_{i+} - z_{i-})$, $\breve{x}_{i0} \in X_{i\varepsilon_i}$, $\breve{z}_{i0} \in Z_{i\epsilon_i}$, $\breve{u}_{i0} \in U_{i0}$ and $\breve{p}_{i0} \in P$. Set $\breve{w}_{i0} \doteq (\breve{x}_{i0}^T, \breve{z}_{i0}^T, \breve{u}_{i0}^T, \breve{p}_{i0}^T)^T$, and $\breve{w}_0 = (\breve{w}_{00}^T, \breve{w}_{10}^T, ..., \breve{w}_{j0}^T)^T$ and $k = 0$.

Step 1: If $k = l$ go to *Step 4*. Else determine the differential and algebraic state trajectories $\widetilde{x}_{ik}$ and $\widetilde{z}_{ik}$ by the shot in the kth time interval for a given layer shooting optimization variable w_k.

Step 2: Using the results of the current shot determine

- the consecutive shooting differential states $\breve{x}_{i,k+1,n} = \varepsilon_{in} + x_{in-}$ if $\widetilde{x}_{ikn}(t_{k+1}) \le \varepsilon_{in} + x_{in-}$, and $\breve{x}_{i,k+1,n} = \widetilde{x}_{ikn}(t_{k+1})$ if $\widetilde{x}_{ikn}(t_{k+1}) \in (\varepsilon_{in} + x_{in-}, -\varepsilon_{in} + x_{in+})$, and $\breve{x}_{i,k+1,n} = -\varepsilon_{in} + x_{in+}$ if $\widetilde{x}_{ikn}(t_{k+1}) \ge -\varepsilon_{in} + x_{in+}$ $(i = 0, 1, ..., j;\ n = 1, 2, ..., n_x)$,
- the consecutive shooting algebraic states $\breve{z}_{i,k+1,n} = \epsilon_{in} + z_{in-}$ if $\widetilde{z}_{ikn}(t_{k+1}) \le \varepsilon_{in} + z_{in-}$, and $\breve{z}_{i,k+1,n} = \widetilde{z}_{ikn}(t_{k+1})$ if $\widetilde{z}_{ikn}(t_{k+1}) \in (\varepsilon_{in} + z_{in-}, -\varepsilon_{in} + z_{in+})$, and $\breve{z}_{i,k+1,n} = -\varepsilon_{in} + z_{in+}$ if $\widetilde{z}_{ikn}(t_{k+1}) \ge -\varepsilon_{in} + z_{in+}$ $(i = 0, 1, ..., j;\ n = 1, 2, ..., n_z)$, and choose the consecutive shooting controls $\breve{u}_{i,k+1} \in U_{i,k+1}$ $(i = 0, 1, ..., j)$, and the consecutive shooting parameters $\breve{p}_{i,k+1} = \breve{p}_{ik}$, and denote the solution found for the consecutive interval as $\breve{w}_{k+1} \doteq (\breve{x}_{k+1}^T, \breve{z}_{k+1}^T, \breve{u}_{k+1}^T, \breve{p}_{k+1}^T)^T$.

Step 3: Determine

- the defect functions of the shooting differential states $G_{1ikn}(w) \doteq \widetilde{x}_{ikn}(t_{k+1}) - x_{i,k+1,n}$ if $\widetilde{x}_{ikn}(t_{k+1}) \le \varepsilon_{in} + x_{in-}$ or $\widetilde{x}_{ikn}(t_{k+1}) \in (\varepsilon_{in} + x_{in-}, -\varepsilon_{in} + x_{in+})$, and $G_{1ikn}(w) \doteq -\widetilde{x}_{ikn}(t_{k+1}) + x_{i,k+1,n}$ if $\widetilde{x}_{ikn}(t_{k+1}) \ge -\varepsilon_{in} + x_{in+}$ $(i = 0, 1, ..., j;\ n = 1, 2, ..., n_x)$,
- the defect functions of the consistency for the algebraic states and the boundary conditions $G_{2ikn}(w) \doteq g_{ikn}(x_{ik}, z_{ik}, u_{ik}, p_{ik})$ if $g_{ikn}(x_{ik}, z_{ik}, u_{ik}, p_{ik}) \le 0$, and $G_{2ikn}(w) \doteq -g_{ikn}(x_{ik}, z_{ik}, u_{ik}, p_{ik})$ in the opposite case $(i = 0, 1, ..., j;\ n = 1, 2, ..., n_z)$,
- the defect functions for the discretized parameter $G_{3ikn}(w) \doteq p_{ik} - p_{i,k+1}$. Set $k = k + 1$.

Step 4: Determine the defect functions for the technological constraints

$$G_{jln}(w) \doteq \sum_{k=0}^{l-1} \int_{t_k}^{t_{k+1}} \tilde{h}(\widetilde{x}_{jk}(t), \widetilde{z}_{jk}(t), \widetilde{u}_{0k}(t), p_{jk})$$

if

$$\sum_{k=0}^{l-1} \int_{t_k}^{t_{k+1}} \tilde{h}(\widetilde{x}_{jk}(t), \widetilde{z}_{jk}(t), \widetilde{u}_{0k}(t), p_{jk}) \le 0,$$

and

$$G_{jln}(w) \doteq -\sum_{k=0}^{l-1} \int_{t_k}^{t_{k+1}} \tilde{h}(\widetilde{x}_{jk}(t), \widetilde{z}_{jk}(t), \widetilde{u}_{0k}(t), p_{jk})$$

in the opposite case $(n = 1, 2, ..., n_{\tilde{h}})$. Save the solution found as $\breve{w} \doteq (\breve{w}_1^T, \breve{w}_2^T, ..., \breve{w}_l^T)^T$.

Step 5: Set up the functions required for the formulation of the MSD$_c$ problem:

$$G_{1ik}(w) \doteq (G_{1ikn}(w))_{n=1}^{n_x},\ \ G_{2ik}(w) \doteq (G_{2ikn}(w))_{n=1}^{n_z},$$

$$G_{3ik}(w) \doteq (G_{3ikn}(w))_{n=1}^{n_p},$$

$$G_{ik}(w) \doteq (G_{1ik}^T(w), G_{2ik}^T(w), G_{3ik}^T(w))^T,$$

$$G_{jl}(w) \doteq (G_{jln}(w))_{n=1}^{n_{\tilde{h}}},$$

$$G_{j+1+i,\,l+1+k}(w) \doteq (-w_{ik}^T + w_{ik-}^T, w_{ik}^T - w_{ik+}^T)^T,$$

$$w_{ik\pm} \doteq (x_{i\pm}^T, z_{i\pm}^T, u_{k\pm}^T, p_\pm^T)^T \ \ (i = 0, 1, ..., j; k = 0, 1, .., l).$$

Step 6: State the converted problem (the c-problem): minimize the objective function

$$J_c(w) \doteq J(w) - c \sum_{i=0}^{j} \sum_{k=0}^{l} G_{ik}(w) \tag{13}$$

subject to the constraints

$$G_{ik}(w) \le 0 \ \ (i = 0, 1, ..., 2j+1; k = 0, 1, ..., 2l+1). \tag{14}$$

where $c \in R_+$ is the cost coefficient of the problem conversion.

If the coefficient c is sufficiently large the discretized problem and the c-problem have the same KKT points [8],[7],[15]. *Algorithm 1* yields by its formulation a feasible solution $\breve{w}$ of the c-problem, which can be further assumed as an initial solution $w^0 \doteq \breve{w}$ for efficient feasible-SQP type algorithms solving this problem. The issues connected with a suitable choice of the coefficient c, and with the verification of the feasibility of the MSPD problem (and eventually of the PD problem) by an optimal solution of the MSPD$_c$ problem are taken up by

Algorithm 2: The search for a locally optimal solution w^* of the MSPD problem and for a locally suboptimal layer solution $(x_i^*, z_i^*, u_i^*, u_{0i}^*, p_i^*)$ of the PD problem by the time-space multipoint shooting feasible-SQP (TMSFSQP) method.

Step 0: Input the initial solution w^0 found by *Algorithm 1*, a symmetric positive definite matrix $H \in R^{n_w \times n_w}$, and positive constants $c_0, \bar{c}, \varrho > 1$ and $\bar{\varrho} \in (0, 1)$.

Step 1: To find a locally optimal solution w^* of the MSD_c problem use the Matlab R2010b feasible-SQP active set procedure solving the compatible equality constrained QP subproblems of the form

$$J'_{c,w}(w)d + \frac{1}{2}d^T H(w)d$$

s.t.

$$G'_{ik,w}(w)d = b(w) \ \ (i,k) \in \mathcal{A}_\kappa(w),$$

where $\mathcal{A}_\kappa(w)$ is an estimate of the active set. Determine the Lagrange multipliers $\lambda_{ik}(c)$ associated with the constraints $G_{ik}(w)$ $(i = 0, 1, ..., j;\ k = 0, 1, ..., l)$.

Step 2: If $c < \lambda_+ \doteq max\{\lambda_{ik}(w(c))|_\infty, i = 0, 1, ..., j; k = 0, 1, ..., l\}$ set $c := \lambda_+ + \bar{c}$ and return to *Step 1*.

Step 3: If $\sum_{i=0}^{j}\sum_{k=0}^{l} |G_{ik}(w(c))|_\infty = 0$ set $w^* = w(c)$. Else set $c := c + \bar{c}$.

Step 4: If the bound constraints (6) for the differential states $\widetilde{x}_{ik}(t, w^*)$ and for the algebraic states $\widetilde{z}_{ik}(t, w^*)$, $t \in [t_k, t_{k+1}]$, $(i = 0, 1, ..., j;\ k = 0, 1, ..., l-1)$ are satisfied determine a locally suboptimal layer solution of the PD problem as $x^*_{ik}(t) = \widetilde{x}_{ik}(t, w^*)$, $z^*_{ik}(t) = \widetilde{z}_{ik}(t, w^*)$, $u^*_{ik}(t) = \widetilde{u}_{ik}(t, w^*)$, $p^*_{ik}(t) = \widetilde{p}_{ik}(t, w^*)$, $t \in [t_k, t_{k+1}]$, $(i = 0, 1, ..., j; k = 0, 1, ..., l-1)$. Else set $\varepsilon := \varrho\varepsilon$ and $\epsilon := \varrho\epsilon$ and go to *Step 0*.

The algorithm exploits the equivalence of the KKT points of the MSPD_c and MSPD problems for sufficiently large c, which should exceed the maximum modulus of the Lagrange multipliers for the converted constraints $G_{ik}(w)$ $(k = 0, 1, ..., l)$ (the c-condition). If this condition is violated the coefficient c is increased (*Step 2*), and the optimization process is repeated. Else the fulfilling of the equality constraints of the MSPD problem is verified. It can be violated even if the c-condition is satisfied for numerical errors propagation in large-scale PDAE systems. Then some further increase of the coefficient c may be helpful (*Step 3*). The violation of the bound constraints for the differential and algebraic states can be removed by the manipulation of the parameters ε and ϵ in view of the calmness of the layer DAE systems under discussion [12]. This leads to a locally suboptimal layer solution of the basic PD problem (*Step 4*).

The computational experience showed that the coefficient c may be overestimated leading to the ill-conditioning of the optimization problem (see fig.1). Thus the practical approach for the finding of the proper value of c may require its decrease and the repeated application of Algorithm 2 as for complex problems such as the optimization of PDAE systems.

We illustrate the theoretical considerations by the heat transfer problem for the probe heating the object with difficult accessibility, and by the performance optimization problem for chemical production processes.

Example 1: Consider the heat transfer process for the probe heating the object with difficult accessibility. The desired temperature profile at the right boundary of the probe should be reached avoiding overheating the zone at its left boundary, where the controlled heat source is exploited. We search for a boundary control u_0 minimizing the objective function

$$\int_0^\tau (x(t,1) - \xi(t))^2 dt + \rho \int_0^\tau u_0^2(t)dt \qquad (15)$$

subject to the heat transfer diffusion state equation

$$C(x(t,s))x_t(t,s) = Dx_{ss}(t,s), \ \ (t,s) \in \Omega_\tau$$

to the initial temperature distribution

$$x(0,s) = x_0(s), \ \ s \in I,$$

to the boundary conditions

$$Dx_s(t,0) = \gamma(x(t,0) - u_0(t)), \ \ Dx_s(t,1) = 0, \ \ t \in I_\tau,$$

and to the spatially sensitive state constraints

$$x(t,s) \le x_+(s), \ \ (t,s) \in \Omega_\tau,$$

where $x(t,s)$ is the temperature along the probe, $u_0(t)$ is the boundary heating control, $\xi(t)$ is the desired temperature profile, ρ is the heating cost coefficient, $C(x(t,s)) \doteq \alpha + \beta x(t,s)$ is the temperature dependent heat capacity of the probe, D is the diffusion coefficient, $x_+(s) \doteq a + bs$, and α, β, γ, a and b are positive constants. The problem is normalized to the form: minimize

$$\int_0^1 (x(t,1) - \xi(t))^2 dt + \rho \int_0^1 u_0^2(t)dt$$

s.t.

$$x_t(t,s) = Dx_{ss}(t,s)/(\alpha + \beta x(t,s)), \ \ (t,s) \in \Omega$$

$$x(0,s) = x_0(s), \ \ s \in I,$$

$$x_s(t,0) = \tilde{\gamma}(x(t,0) - u_0(t)), \ \ x_s(t,1) = 0, \ \ t \in I,$$

$$x(t,s) \le a + bs, \ \ (t,s) \in \Omega.$$

The distributed parameter model is approximated in each time interval $[t_k, t_{k+1}]$ by the system of ordinary differential equations for $i = 1, 2, ..., j$

$$\dot{\widetilde{x}}_{ik}(t) = D_j(\widetilde{x}_{i+1,k}(t) - 2\widetilde{x}_{ik}(t) + \widetilde{x}_{i-1,k}(t))/(\alpha + \beta\widetilde{x}_{ik}(t)),$$

and by algebraic equation following from the approximation of the left boundary condition

$$\widetilde{x}_{1k}(t) = \tilde{\gamma}(\widetilde{x}_{0k}(t) - \widetilde{u}_{0k}(t)),$$

where $D_j \doteq D/\delta_j^2$, $\delta_j \doteq 1/j$. The right boundary condition determines the variable $\widetilde{x}_{j+1,k}(t)$ as $\widetilde{x}_{j+1,k}(t) \doteq \widetilde{x}_{jk}(t)$. The initial conditions are determined by the shooting variables as follows

$$\widetilde{x}_{ik}(t_k) = x_{ik} \ \ (i = 0, 1, 2, ..., j).$$

Thus the shot in each interval $[t_k, t_{k+1}]$ is reduced to the solving of a large-scale DAE system approximating the basic PDAE system. The distinctive features of the above example encompass the spatially dependent state constraints, the potential instabilities in the process nonlinear model caused by high sensitivity of the heat capacity to the large variations of the temperature in the probe, and the sparse structure of

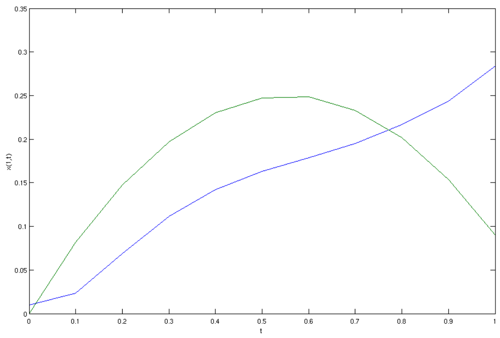

Figure 1. Too high c

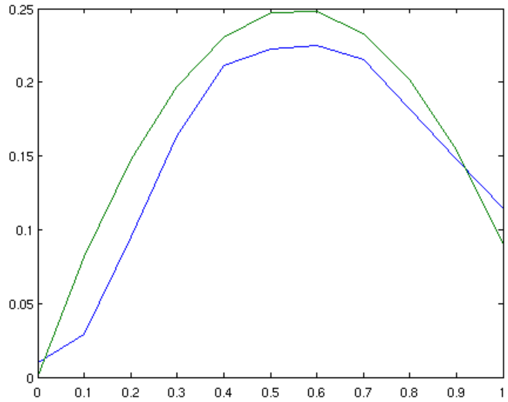

Figure 2. Resulting temperature profile

the approximating DAE system, which can be advantageously exploited in the solution procedure.

In *Example 1* let's consider $\xi(t) = 0.9t - 0.81t^2$. For simplicity we use small number of equations $j = 5$ and small number of shots $l = 5$. We use the initial condition $x_{ik} = (0.01\ 0.01\ 0.01\ 0.01\ 0.01)$.

The results of calculations are good but not astonishing. First of all the results depends on the coefficient c. When it is too small, the equality constrains aren't satisfied. When it is too high, the constrains are satisfied, but high ratio of penalty to square error of right boundary gives disappointing results for the desired temperature profile shown on fig. 1. We have chosen $\rho = 0.3$, $c = 0.1$. It is giving fair result, shown on fig. 2. Optimal boundary control and optimal state surface are shown on fig.3 and fig.4.

Example 2: Consider the chemical production process performed in a tubular reactor. The averaged gain from the conversion of the raw material A into the desired product B at the outlet of the reactor should be maximized avoiding excessive concentrations of A in the initial zone of the reactor, which may lead to the undesirable catalyst poisoning. We search for a boundary control $u_0(t)$, for a distributed control $u(t, s)$, and for a global parameter p minimizing the objective

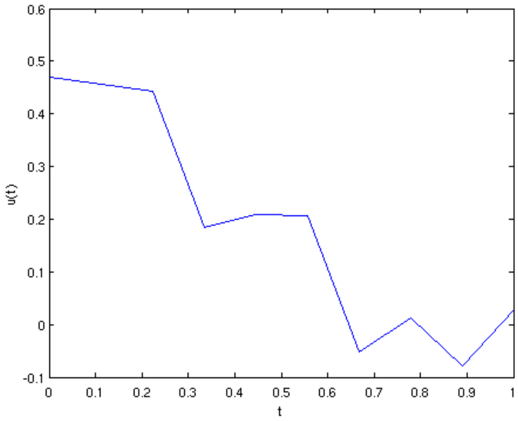

Figure 3. Optimal boundary control profile

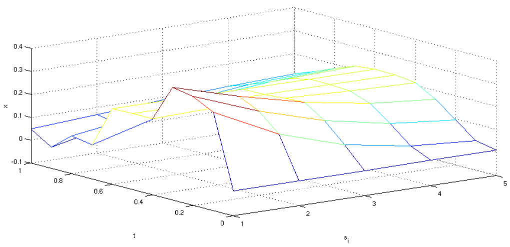

Figure 4. Time-space optimal state trajectory

function

$$\int_0^1 (x(t, 1) + \rho u_0(t))dt$$

subject to the mass transfer diffusion-convexion state equation

$$x_t(t, s) = Dx_{ss}(t, s) - u(t, s)x_s(t, s) - \kappa(p)x^{\alpha}(t, s), (t, s) \in \Omega,$$

to the initial distribution of A

$$x(0, s) = x_0(s), \quad s \in I,$$

to the boundary conditions

$$Dx_s(t, 0) = v(t, 0)(x(t, 0) - u_0(t)), \quad Dx_s(t, 1) = 0, \quad t \in I,$$

and to the state and control box constraints

$$x(t, s) \in [0, x_+(s)], \quad u(t, s) \in [0, u_+], \quad (t, s) \in \Omega,$$

$$u_0(t) \in [0, u_{0+}], \quad t \in I,$$

where $x(t, s)$ is the concentration of A in the reactor, $u_0(t)$ is the inlet concentration of A, $u(t, s)$ is the time-space variable flow intensity of the reacting mixture, p is the process temperature, $\kappa(p) \doteq \kappa_0 e^{-\beta/p}$ is the Arrhenius function, and α is the reaction order.

The distributed parameter model is approximated in each time interval $[t_k, t_{k+1}]$ by the system of ordinary differential equations for $i = 1, 2, ..., j$

$$\dot{\tilde{x}}_{ik}(t) = D_j(\tilde{x}_{i+1,k}(t) - 2\tilde{x}_{ik}(t) + \tilde{x}_{i-1,k}(t))$$

$$(-\widetilde{u}_{ik}(t)(\widetilde{x}_{i+1,k}(t)-\widetilde{x}_{ik}(t))+\kappa(p)\widetilde{x}_{ik}^{\alpha}(t))/\delta_j,$$

and by algebraic equation following from the approximation of the left boundary condition

$$\widetilde{x}_{1k}(t)=\tilde{\gamma}\widetilde{u}_{0k2}(t)(\widetilde{x}_{0k}(t)-\widetilde{u}_{0k1}(t)),$$

where $D_j \doteq D/\delta_j^2,\ \delta_j \doteq 1/j$. The right boundary condition determines the variable $\widetilde{x}_{j+1,k}(t)$ as $\widetilde{x}_{j+1,k}(t) \doteq \widetilde{x}_{jk}(t)$. The initial conditions are determined by the shooting variables as follows

$$\widetilde{x}_{ik}(t_k)=x_{ik}\ \ (i=0,1,2,...,j).$$

Thus the shot in each interval $[t_k, t_{k+1}]$ is reduced as in *Example 1* to the solving of a large-scale DAE system approximating the basic PDAE system. Denoting by $z(t,s)$ the concentration of the desired product as the algebraic state variable satifying the algebraic equations

$$x(t,s)+z(t,s)=1,\ \ (t,s)\in\Omega,$$

we can formulate the technological constraint as the demand of the prescribed amount $\bar{z}$ of the desired product at the outlet of the reactor in the interval $(0,1)$

$$\int_0^1 z(t,1)dt=\bar{z}.$$

The distinctive features of the above example encompass the spatially dependent state constraints, the potential instabilities in the process nonlinear model caused by high sensitivity of the reaction rate to the large variations of the temperature and the concentration of A, and the sparse structure of the approximating DAE system, which can be advantageously exploited in the solution procedure.

IV. Conclusion

We presented multipoint shooting algorithms specialized to the optimization of parabolic DAE systems. They use the feasible-SQP method, which aims at the finding of a suboptimal solution of a high practical applicability. We described a procedure of obtaining an initial feasible solution for the multipoint shooting problem exploiting the results of consecutive shots of the system trajectory. We emphasized the specific features of the proposed approach such as the spatially sensitive state constraints, the potential instabilities in the discussed heat and mass transfer processes, and the sparse structure of the large-scale DAE systems approximating the basic partial differential equations.

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