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ON SOLVING OPTIMIZATION-CONSTRAINED DIFFERENTIAL EQUATIONS BY USING KKT CONDITIONS

XIAO ZHAO

IBG-1, Biotechnology, Forschungszentrum Juelich GmbH
52425 Juelich, Germany, x.zhao@fz-juelich.de

ABSTRACT. The work studies the theoretical solution of optimization-constrained differential equations (OCDE) and proposes a numerical algorithm to solve it. Regularity conditions are given such that OCDE can be locally transformed into index-1 differential algebraic equation (DAE) systems. At non-regular points, where strict complementarity condition is damaged, we study the switching behavior of OCDE. Conditions are given at these non-regular points, such that one can construct a new DAE system and continue simulation from there. To exactly locate the switching time, i.e. where strict complementarity condition is damaged, an event function is proposed. Under transversality conditions the proposed event function changes its sign. Two examples are provided to illustrate the solution approach.

Key Words Optimization-constrained differential equations, Parametric optimization, Hybrid dynamic system, Switching behavior, Solution algorithm.

1. INTRODUCTION

For $x \in \mathbb{R}^{n_x}$, $v \in \mathbb{R}^{n_v}$, denote $P(x)$ as a parametric optimization [5, 10, 8, 9], which takes the form of

$$\min_{v} \; g(x,v) \tag{1.1a}$$

$$s.t. \; h_i(x,v) = 0, \quad i = 1, \ldots, N, \tag{1.1b}$$

$$l_j(x,v) \geq 0, \quad j = 1, \ldots, M. \tag{1.1c}$$

N and M are fixed integers. $g : \mathbb{R}^{n_x} \times \mathbb{R}^{n_v} \to \mathbb{R}$, $h_i : \mathbb{R}^{n_x} \times \mathbb{R}^{n_v} \to \mathbb{R}$, $l_j : \mathbb{R}^{n_x} \times \mathbb{R}^{n_v} \to \mathbb{R}$ are sufficiently smooth functions. For each fixed $x = \bar{x}$, $P(\bar{x})$ looks for the local minimums of the objective function $g(\bar{x}, v)$ subjected to constraints (1.1b)–(1.1c), which are evaluated at $x = \bar{x}$. We say that optimization problem $P(x)$ is parametrized by x.

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In this work, we consider solving the so-called optimization-constrained differential equations (OCDE), which takes the form of

$$\dot{x} = f(x, v), \quad x(0) = x_0, \tag{1.2a}$$

$$v \in \{v \in \mathbb{R}^{n_v} \mid v \text{ is a local minimizer of } P(x)\}. \tag{1.2b}$$

$f : \mathbb{R}^{n_x} \times \mathbb{R}^{n_v} \to \mathbb{R}^{n_x}$ is a sufficiently smooth function. By $\dot{x}$ we mean that $dx(t)/dt$, where x is a function of time t, $t \geq 0$. $x_0 \in \mathbb{R}^{n_x}$ denotes the initial condition at $t = 0$. Eq. (1.2) contains an upper level part (1.2a), which corresponds to a classical ordinary differential equations (ODE), and a lower level part (1.2b), which is a parametric optimization. Because of the bi-level structure of Eq. (1.2), solving OCDE (1.2) requires to solve the inner optimization problem $P(x(t))$, $\forall t \geq 0$.

In the literature, there exist already some works which use system (1.2) to model and simulate technical systems. Landry et al. [13] present an OCDE model for the simulation of dynamic phase transition for a single atmospheric aerosol particle that exchanges mass with surrounding gas. They use Karush-Kuhn-Tucker (KKT) optimality condition to reformulate the inner optimization problem and develop a mechanism to detect the discontinuity caused by activation and deactivation of inequality constraints. Caboussat and Landry [1], Caboussat et al. [2] consider similar applications, but propose a numerical method based on an operator splitting scheme and a fixed point algorithm. Kaplan et al. [11] apply the OCDE framework in modeling and simulating metabolic networks for the estimation of biomass accumulation parameters. Their solution approach is based on the approximated KKT conditions. The OCDE framework is also used in cybernetic modeling of microbial growth [19], which is based on the understanding that cells make "rational" (optimal) decisions in responding to its environment. Recently, Harwood et al. [6], Hoeffner et al. [7] propose the so-called dynamic flux balance approach, in which the OCDE formulation includes a lexicographic linear programming.

Because solving OCDE requires that for each $t \geq 0$, one solves problem $P(x(t))$, parametric optimization is a closely related topic. General reviews of parametric optimization can be found in [4, 8]. Consider the parametric optimization problem $P(x)$ defined in Eq. (1.1), if we assume that local minimizers of $P(x)$ are locally unique, we can denote the optimal solution of $P(x)$ by $v^*(x)$, where $v^*(\cdot)$ is an implicitly defined function. One of the important questions of parametric optimization is to ask, how does the function $v^*(\cdot)$ looks like? For example, is it locally smooth? This question is important to study the theoretical solutions of OCDE (1.2), because if such function is known, one can directly replace $v = v^*(x)$ in Eq. (1.2a), which results in an ordinary differential equation (ODE)

$$\dot{x} = f(x, v^*(x)), x(0) = x_0. \tag{1.3}$$

However, we need to note that the right hand side of Eq. (1.3) may not be smooth, because function $v^*(\cdot)$ may be nonsmooth.

The question of local smoothness of function $v^*(\cdot)$ is already studied by the stability issue of parametric optimization. It is shown that, function $v^*(\cdot)$ may show non-smooth behavior, i.e. continuous (but non-smooth) or discontinuous, for smooth functions g, h_i and l_j [4]. Simple examples of this situation are presented in [10]. To author's knowledge, the discussion of the stability issue can be roughly classified into two categories: results based on the application of the Implicit Function Theorem (IFT), refer to Theorem 1 in the appendix, and results where the IFT is not applicable. Generally speaking, IFT-based results are easier to follow, which lead directly to the smoothness of function $v^*(\cdot)$. Non-IFT-based results are more difficult. This paper will restrict the discussion to IFT-based results.

The major contribution of this work is to study the theoretical solutions of OCDE (1.2) by applying the results of parametric optimization. We formulate sufficient conditions such that OCDE (1.2) can be locally transformed into a smooth index-1 DAE system at regular points. At non-regular points, where sufficient conditions are damaged, switching behavior of OCDE (1.2) is observed and analyzed. At these points, we define new DAE systems and propose transversality conditions such that solution of the original OCDE can be continued. To locate switching points, an event function is proposed, which can implemented straightforwardly in numerical DAE solvers. A numerical algorithm for OCDE is presented at the end.

In comparison to the work [13], our results are based on a more general nonlinear formulation of OCDE (1.2), while the discussion there is oriented to a special application. We give sufficient conditions, such that the solution of OCDE can be described by DAE systems both at regular and non-regular switching points. Transversality condition is proposed to study the switching behavior and a numerical algorithm for OCDE is proposed at the end. In comparison to the work [6, 7], we consider a nonlinear inner optimization problem and use KKT-based reformulation, which leads to a less restrictive approach. We have to note that, more complicated behaviors of OCDE, e.g. vanish/born of local minimizer, appearance of limits points, refer to the examples in [10], are not covered in this work. The studied switching behavior is only one type of singularity behaviors when solving OCDE. Studying more complicated behaviors of OCDE remains an open question in the future.

The paper is organized as follows. In Section 2, we review the relevant results of parametric optimization. In Section 3 we talk about the solution method of OCDE, based on the presented results so far. In Section 4, we present two numerical examples, one of which comes from systems biotechnology.

2. PARAMETRIZED KKT CONDITIONS

This section discusses the usage of Karush Kuhn Tucker (KKT) conditions (also known as the Kuhn Tucker conditions) to characterize and tract local minimizers of $P(x)$. The presented results are based on the work of [10, 9, 8, 5, 4], which are reorganized to fit to the discussion of this paper. Parametrized KKT conditions will be used later to transform OCDE (1.2) into differential-algebraic equation (DAE) systems, which can be solved by classical DAE solvers.

Denote $I = \{1, \dots, N\}$ and $J = \{1, \dots, M\}$ as the index sets for equality and inequality constraints of $P(x)$, respectively. For any fixed point x, denote

$$\mathcal{M}_x = \{v \in \mathbb{R}^{n_v} \mid h_i(x, v) = 0, i \in I, l_j(x, v) \geq 0, j \in J\} \tag{2.1}$$

as the feasible set of $P(x)$. Denote

$$\mathcal{A}(x, v) = \{j \in J \mid l_j(x, v) = 0\} \tag{2.2}$$

as the index set of active inequality constraints, which is evaluated at point $(x^T, v^T)^T$. $\mathcal{A}(x, v)$ is also called the active set of $P(x)$, evaluated at v. Define

$$L(x, v, \lambda, \mu) = g(x, v) + \sum_{i \in I} \lambda_i h_i(x, v) - \sum_{j \in J} \mu_j l_j(x, v) \tag{2.3}$$

as the Lagrangian function of $P(x)$, where $\lambda_i \in \mathbb{R}$, $i \in I$, and $\mu_j \in \mathbb{R}$, $j \in J$. Denote $\lambda := (\lambda_1, \dots, \lambda_N)^T \in \mathbb{R}^N$ and $\mu := (\mu_1, \dots, \mu_M)^T \in \mathbb{R}^M$. λ and μ are called Lagrangian multipliers for equality and inequality constraints, respectively. To simplify notation, we denote $z = (v^T, \lambda^T, \mu^T)^T$.

For any given subset J^* of J, i.e. $J^* \subseteq J$, define function

$$F_{J^*}(x, v, \lambda, \mu) = \begin{pmatrix} \nabla_v L^T(x, v, \lambda, \mu) \\ h_i(x, v), \forall i \in I \\ -l_j(x, v), \forall j \in J^* \\ \mu_j, \forall j \notin J^* \end{pmatrix}. \tag{2.4}$$

$\nabla_v L \in \mathbb{R}^{1 \times n_v}$ refers to a row vector. Therefore, by choosing different subsets $J^* \subseteq J$, we can obtain different functions $F_{J^*}(\cdot)$. For example, a special case of F_{J^*} is $F_{\mathcal{A}(\bar{x}, \bar{v})}$, which is obtained by choosing $J^* = \mathcal{A}(x, v)|_{x = \bar{x}, v = \bar{v}}$.

Definition 2.1 (LICQ)**.** For fixed $x = \bar{x}$, linear independence constraint qualification (LICQ) is said to hold for $P(\bar{x})$ at $v = \bar{v}$, if the vectors $\nabla_v h_i(\bar{x}, \bar{v})$, $i \in I$, $\nabla_v l_j(\bar{x}, \bar{v})$, $j \in \mathcal{A}(\bar{x}, \bar{v})$ are linearly independent.

Note that there exist other constraint qualifications (CQ) [17], e.g. MFCQ [14] and SMFCQ [12]. LICQ is stronger than MFCQ and SMFCQ, and in this work we only need the definition of LICQ.

It is well known that under suitable CQ, e.g. LICQ, there exist Lagrangian multipliers such that $F_{J^*=\mathcal{A}(\bar{x},\bar{v})}=0$ holds at local minimums of $P(x)$. We state this result formally for completeness.

Theorem 2.2 (First order necessary optimality condition, refer to e.g. Theorem 12.1 in [15])**.** *For fixed $x=\bar{x}$, if v^* is a local minimum of $P(\bar{x})$ and if LICQ holds at $v=v^*$, then there exist $\lambda^*\in\mathbb{R}^N$ and $\mu^*\in\mathbb{R}^M$, such that*

$$0=F_{\mathcal{A}(x,v)}(x,v,\lambda,\mu), \tag{2.5a}$$

$$0\le l_j(x,v),\quad \forall j\in J, \tag{2.5b}$$

$$0\le \mu_j,\quad \forall j\in J, \tag{2.5c}$$

hold, for $x=\bar{x}$, $v=v^*$, $\lambda=\lambda^*$ and $\mu=\mu^*$.

We note that Eq. (2.5a) is said to hold for $x=\bar{x}$, $v=v^*$, $\lambda=\lambda^*$ and $\mu=\mu^*$, if

$$0=F_{\mathcal{A}(\bar{x},v^*)}(\bar{x},v^*,\lambda^*,\mu^*). \tag{2.6}$$

Eq. (2.5) is the so-called KKT necessary optimality condition of $P(x)$. At $x=\bar{x}$, vector $z^*=(v^{*T},\lambda^{*T},\mu^{*T})^T$ is called a KKT point of $P(\bar{x})$, if z^* satisfies Eq. (2.5). From Theorem 2.2, roughly speaking, the task of finding local minimums can be transformed to finding the solutions of Eq. (2.5), i.e. finding KKT points.

We note that, Theorem 2.2 provides a necessary condition for local minimizers. It is obvious that some KKT points may not be local minimums, e.g. a saddle point. To guarantee that KKT points are local minimums, we state a second order sufficient condition, which will be used later.

Definition 2.3 (Strict complementarity (SC) condition)**.** For fixed $x=\bar{x}$, assume that $z^*=(v^{*T},\lambda^{*T},\mu^{*T})^T$ is a KKT point of $P(\bar{x})$, i.e. $\bar{x}$, z^* satisfy Eq. (2.5), we say that strict complementarity (SC) condition holds for $z=z^*$, if

$$\mu_j^*>0,\quad \forall j\in\mathcal{A}(\bar{x},v^*). \tag{2.7}$$

In other words, SC condition requires that Eq. (2.5c) strictly holds for all active inequality constraints.

Let H be any symmetric $n\times n$ real matrix and $T\subset\mathbb{R}^n$ be a linear space. By $H|_T$ we mean some matrix in the family

$$\mathcal{V}=\{V^THV \mid V \text{ is matrix with } n \text{ rows,}$$
$$\text{whose columns form a basis of space } T\},$$

refer to [10]. It is known that, the numbers of positive, zero and negative eigenvalues of V^THV do not depend on the specific choice of V. Therefore, the numbers of positive, zero and negative eigenvalue of $H|_T$ can be defined according to the correspond numbers of $V^T HV$ [10]. For example, $H|_T$ is said to be non-singular (positive definite), if matrix $V^T HV$ is non-singular (positive definite).

For any $n \times m$ matrix A, $KerA := \{y \in \mathbb{R}^m \mid Ay = 0\}$ denotes the kernel of A. For fixed $x = \bar{x}$, denote $T_{v^*}\mathcal{M}_{\bar{x}}$ as the tangent space of the feasible set $\mathcal{M}_{\bar{x}}$ at $v = v^*$, i.e.

$$\begin{aligned} T_{v^*}\mathcal{M}_{\bar{x}} :&= \bigcap_{i\in I} Ker\nabla_v h_i(\bar{x}, v^*) \cap \bigcap_{j\in\mathcal{A}(\bar{x},v^*)} Ker\nabla_v l_j(\bar{x}, v^*) \\ &= Ker\ [\underbrace{\ldots, \nabla_v^T h_i(\bar{x}, v^*), \ldots}_{i\in I}, \underbrace{\ldots, \nabla_v^T l_j(\bar{x}, v^*), \ldots}_{j\in\mathcal{A}(\bar{x},v^*)}]^T. \end{aligned} \tag{2.8}$$

$T_{v^*}\mathcal{M}_{\bar{x}}$ is therefore a linear subspace of $\mathbb{R}^{n_v}$.

Theorem 2.4 (Second order sufficient optimality condition, refer to Lemma 3.2.1 in [4])**.** *For fixed $x = \bar{x}$, if there exists point $z^* = (v^{*T}, \lambda^{*T}, \mu^{*T})^T$ such that Eq.* (2.5) *and SC condition hold, and if*

$$\nabla_v^2 L(\bar{x}, v^*, \lambda^*, \mu^*)|_{T_{v^*}\mathcal{M}_{\bar{x}}} \text{ is positive definite,} \tag{2.9}$$

then v^* is a strict local minimum of $P(x^*)$, i.e. there exists a neighborhood of v^* such that there does not exist any feasible $v' \neq v^*$ such that $g(\bar{x}, v') \leq g(\bar{x}, v^*)$.

In the previous discussions, we have talked about the optimality conditions of $P(x)$ at a given fixed point $x = \bar{x}$. Next, in order to study the dependence of local minimums v^* on x, i.e. function $v^*(\cdot)$, we will consider an unfixed point x. We note that, although studying the dependence of local minimum points v^* on x is desirable, in the following text we will restrict to study the dependence of KKT points (which may or may not be local minimizers) on variable x. The discussion can be adapted to local minimum points, if one assumes that the conditions in Theorem 2.4 hold.

To study the local dependence of KKT points on x, let us firstly give a lemma about Eq. (2.4). This lemma is frequently accessed later in this work. $\forall J^* \subseteq J$, denote

$$B_{J^*}(x, v) = [\underbrace{\ldots, \nabla_v h_i^T, \ldots}_{i\in I}, \underbrace{\ldots, \nabla_v l_j^T, \ldots}_{j\in J^*}] \in \mathbb{R}^{n_v\times(|I|+|J^*|)}$$

as a matrix, whose columns are gradients of equality ($i \in I$) and inequality constraints ($j \in J^*$).

Lemma 2.5 (Non-singularity of $\nabla_z F_{J^*}$, refer to Lemma 1 in the appendix)**.** *For any $J^* \subseteq J$, $\nabla_z F_{J^*}(x, z)$ is non-singular at a point $(x^T, z^T)^T$, if and only if*

$$B_{J^*}(x, v) \text{ has full column rank,} \tag{2.10a}$$

$$\nabla_v^2 L(x, z)|_{KerB_{J^*}^T(x,z)} \text{ is non-singular.} \tag{2.10b}$$

Proof. Apply Lemma 1 to

$$\nabla_z F_{J^*} = \begin{pmatrix} \nabla_v^2 L & \nabla_v h_i^T, i \in I & -\nabla_v l_j^T, j \in J^* & -\nabla_v l_j^T, j \notin J^* \\ \nabla_v h_i, i \in I & 0 & 0 & 0 \\ -\nabla_v l_j, j \in J^* & 0 & 0 & 0 \\ 0 & 0 & 0 & diag(1, \dots, 1)^T \end{pmatrix}.$$

□

Lemma 2.5 has important consequences to our discussions. Consider now that

$$F_{J^*}(x, z) = 0 \tag{2.11}$$

holds at $x = \bar{x}$, $z = \bar{z}$. By applying the IFT, non-singularity of $\nabla_z F_{J^*}(\bar{x}, \bar{z})$ guarantees that there exists a neighborhood $U_{\bar{x}}$ of $\bar{x}$, such that Eq. (2.11) implicitly defines sufficiently smooth functions $v : U_{\bar{x}} \to \mathbb{R}^{n_v}$, $\lambda : U_{\bar{x}} \to \mathbb{R}^N$ and $\mu : U_{\bar{x}} \to \mathbb{R}^M$, satisfying $F_{J^*}(x, v(x), \lambda(x), \mu(x)) \equiv 0$, $\forall x \in U_{\bar{x}}$.

At $x = \bar{x}$, if we consider $z = z^*$ is a KKT point and we choose

$$J^* = \bar{\mathcal{A}} := \mathcal{A}(\bar{x}, v^*), \tag{2.12}$$

in Eq. (2.11), the derived system is denoted as

$$F_{\bar{\mathcal{A}}}(x, z) = 0. \tag{2.13}$$

From Lemma 2.5, it is straightforward to prove that:

Corollary 2.6. *$\nabla_z F_{\bar{\mathcal{A}}}(\bar{x}, z^*)$ is non-singular, if and only if*

$$\text{LICQ holds at } (\bar{x}^T, z^{*T})^T, \tag{2.14a}$$

$$\nabla_v^2 L(\bar{x}, z^*)|_{T_{v^*}\mathcal{M}_{\bar{x}}} \text{ is non-singular.} \tag{2.14b}$$

Proof. If $J^* = \bar{\mathcal{A}}$, $Ker\, B_{J^*}^T(\bar{x}, v^*) = T_{v^*}\mathcal{M}_{\bar{x}}$, refer to Eq. (2.8). □

Denote the solution set of Eq. (2.13) as

$$\Omega_{\bar{\mathcal{A}}} = \{(x^T, v^T)^T \in \mathbb{R}^{n_x + n_v} \mid F_{\bar{\mathcal{A}}}(x, v, \lambda, \mu) = 0\}, \tag{2.15}$$

where $\bar{\mathcal{A}}$ is defined in Eq. (2.12). We have the following lemma which says that in a small neighborhood the active set $\mathcal{A}(x, v)$, for $(x^T, v^T)^T \in \Omega_{\bar{\mathcal{A}}}$, does not change and the feasibility constraints (2.5b)–(2.5c) always hold.

Lemma 2.7. *Consider that $(v^{*T}, \lambda^{*T}, \mu^{*T})^T$ is a KKT point for $x = \bar{x}$, where Conditions* (2.14) *and SC condition hold. Denote $\bar{\mathcal{A}} = \mathcal{A}(\bar{x}, v^*)$ as the active set at $x = \bar{x}$, $z = z^*$. Then there exists a neighborhood U_0 of $(\bar{x}^T, v^{*T})^T$ such that $\forall (x^T, v^T)^T \in U_0 \cap \Omega_{\bar{\mathcal{A}}}$,*

$$\mathcal{A}(x, v) = \bar{\mathcal{A}}, \text{ i.e. the active set does not change }, \tag{2.16a}$$

$$\text{Eqs. (2.5b)–(2.5c) hold.} \tag{2.16b}$$

Proof. From Corollary 2.6 and the IFT, Eq. (2.13) implicitly defines function $v(x)$, $\lambda(x)$ and $\mu(x)$, which are sufficiently smooth. Eq. (2.16a) follows from

$$l_j(\bar{x}, v^*) > 0, \quad j \notin \bar{\mathcal{A}}, \tag{2.17}$$

and the continuity of functions $l_j(\cdot)$ and $v(\cdot)$.

To prove Eq. (2.16b), because of Eq. (2.16a) it is equivalent to prove $\forall (x^T, v^T)^T \in U_0 \cap \Omega_{\bar{\mathcal{A}}}$,

$$0 \le l_j(x, v), \quad \forall j \in \bar{\mathcal{A}}, \tag{2.18a}$$

$$0 \le l_j(x, v), \quad \forall j \notin \bar{\mathcal{A}}, \tag{2.18b}$$

$$0 \le \mu_j, \quad \forall j \in \bar{\mathcal{A}}, \tag{2.18c}$$

$$0 \le \mu_j, \quad \forall j \notin \bar{\mathcal{A}}. \tag{2.18d}$$

Eqs. (2.18a), (2.18d) hold because of the definition of $F_{\bar{\mathcal{A}}}(x, z)$. Eq. (2.18b) holds, because $0 < l_j(\bar{x}, v^*)$, $\forall j \notin \bar{\mathcal{A}}$, and the continuity of $l_j(\cdot)$, $v(\cdot)$. Eq. (2.18c) holds, because of the SC condition $0 < \mu_j^*$, $\forall j \in \bar{\mathcal{A}}$ and the continuity of $\mu(\cdot)$. □

Eq. (2.16a) says that the active set does not change for $\forall (x^T, v^T)^T \in U_0 \cap \Omega_{\bar{\mathcal{A}}}$. Eq. (2.16b) says that the inequality constraints in KKT condition also hold in this region. Therefore, to solve Eq. (2.5) near a given KKT point, one can solve Eq. (2.13) and neglect inequality constraints (2.5b)-(2.5c). This is the main idea of solving OCDE at regular KKT points, refer to Section 3.1. We note here that, one can not directly apply the IFT to Eq. (2.5a), because the subindex $\mathcal{A}(x, v)$ of F is not fixed (In Eq. (2.13) the subindex $\bar{\mathcal{A}}$ is fixed.).

To summarize the consequences of Corollary 2.6 and Lemma 2.7, we have that

Theorem 2.8. *Consider that $(v^{*T}, \lambda^{*T}, \mu^{*T})^T$ is a KKT point for $P(\bar{x})$, if Condition* (2.14) *and SC hold, then there exists a neighborhood $U_{\bar{x}}$ of $\bar{x}$, such that:* (1) *Eq.* (2.13) *implicitly defines sufficiently smooth functions $v : U_{\bar{x}} \to \mathbb{R}^{n_v}$, $\lambda : U_{\bar{x}} \to \mathbb{R}^N$, $\mu : U_{\bar{x}} \to \mathbb{R}^M$.* (2) *$v(\bar{x}) = v^*$, $\lambda(\bar{x}) = \lambda^*$, $\mu(\bar{x}) = \mu^*$.* (3) *$(v(x)^T, \lambda(x)^T, \mu(x)^T)^T$ are KKT points of $P(x)$, $\forall x \in U_{\bar{x}}$, i.e. $(x^T, v(x)^T, \lambda(x)^T, \mu(x)^T)^T$ satisfy Eq.* (2.5)*.*

Note that, because Eq. (2.9) implies Eq. (2.14b), if the other conditions in Theorem 2.8 hold, the derived function $v(x)$ corresponds to strict local minimums. In other words, if the second order sufficient conditions in Theorem 2.4 and LICQ are fulfilled, Eq. (2.13) locally defines smooth functions which correspond to strict local minimums, refer also to Theorem 3.2.2 in [4].

Consider OCDE (1.2) and variable x as a function of time t, Theorem 2.8 suggests a way to locally track the KKT points of $P(x(t))$ by using Eq. (2.13). This property leads to a proposed solution algorithm of OCDE, which will be presented next.

3. SOLUTION METHOD

This section presents a solution method to solve OCDE (1.2). The method is based on the KKT condition (2.5), which transforms an OCDE into a set of DAE systems. In this section, we first talk about solving OCDE under regularity conditions, i.e. under the conditions of Theorem 2.8. After that, we analyze the switching behavior of OCDE, when SC condition is damaged. At the end, we give an algorithm based on the obtained results so far.

3.1. Solving OCDE at regular points.

Definition 3.1 (Regular KKT point)**.** At $x = \bar{x}$, consider $z^* = (v^{*T}, \lambda^{*T}, \mu^{*T})^T$ as a KKT point. This point is called a regular KKT point, if Condition (2.14) and SC condition (2.7) hold.

From Theorem 2.8, we know that the KKT points of $P(x)$ near a given regular KKT point is implicitly defined by Eq. (2.13). Therefore, if we assume that at $x = x_0$, $z^* = (v^{*T}, \lambda^{*T}, \mu^{*T})^T$ is a regular KKT point of $P(x_0)$. To solve OCDE (1.2) starting from $x(0) = x_0$ and $z(0) = z^*$, one can solve the following DAE system

$$\dot{x} = f(x, v), \quad x(0) = x_0, \tag{3.1a}$$

$$0 = F_{\bar{\mathcal{A}}}(x, v, \lambda, \mu), \tag{3.1b}$$

where $\bar{\mathcal{A}} := \mathcal{A}(x_0, v^*)$, as it is defined in Eq. (2.12).

From Corollary 2.6, it can be seen straightforwardly, this DAE system is of index-1. Therefore, DAE (3.1) can be integrated by classical DAE solvers. Note that, the formulation of Eq. (3.1b) requires the determination of set $\bar{\mathcal{A}}$. This can be done by solving $P(x_0)$ using standard nonlinear optimization (NLP) solvers.

3.2. Switching behavior of OCDE at non-regular points.

From the definition of regular KKT points, any violation of Condition (2.14) and/or SC condition (2.7) will cause the KKT points to become non-regular. At non-regular points, because one may not be able to apply the IFT (when Codnition (2.14) is damaged) or continued simulation may violate Eqs. (2.5b), (2.5c) (when SC condition is damaged), KKT points defined by Eq. (2.5) may not smoothly depend on variable x. We note that, a general analysis of this issue is complex, see e.g. [10]. This work is restricted to the case that Condition (2.14) (more exactly, Condition (3.3)) is fulfilled, but SC condition (2.7) is damaged. We note also that the presented discussion in this subsection is motivated by the discussions in [18] and the second type of degenerate points presented in [10]. In comparison to their work, however, this work does not use Fritz John conditions and the SC condition is allowed to be violated for multiple inequality constraints. Moreover, we consider the task of solving OCDE, while the previous-mentioned works do not.

Assume that at $x = \bar{x}^T$, $z^* = (v^{*T}, \lambda^{*T}, \mu^{*T})^T$ is a KKT point corresponding to time $t = \tilde{t}$. Denote

$$\mathcal{S} := \{j \in J \mid \mu_j^* = 0,\ l_j(\bar{x}, v^*) = 0\}$$

as the index set of active inequalities at $t = \tilde{t}$, which do not satisfy SC condition. We have therefore

$$\mathcal{S} \subseteq \mathcal{A}(\bar{x}, v^*) = \bar{\mathcal{A}} \subseteq J,$$

where $\bar{\mathcal{A}}$ denotes the active set of inequalities at $x = \bar{x}$, $v = v^*$. In this work, we consider the non-regular point z^*, for which $\mathcal{S} \neq \emptyset$. That is, SC condition is damaged for $x = \bar{x}$, $z = z^*$.

Denote

$$\Theta = \{\mathcal{S}^* \mid \mathcal{S}^* \text{ is a subset of } \mathcal{S}, \text{ i.e. } \mathcal{S}^* \subseteq \mathcal{S}\}.$$

Because $\mathcal{S}$ contains finite elements, Θ contains also finite elements. $\forall \mathcal{S}^* \in \Theta$ ($\mathcal{S}^*$ may be chosen an empty set), denote $DAE(\bar{\mathcal{A}}/\mathcal{S}^*)$ as the following DAE system

$$\dot{x} = f(x, v), \quad x(\tilde{t}) = \bar{x}, \tag{3.2a}$$

$$0 = F_{\bar{\mathcal{A}}/\mathcal{S}^*}(x, v, \lambda, \mu), \tag{3.2b}$$

where $\bar{\mathcal{A}}/\mathcal{S}^* := \{j \in J \mid j \in \bar{\mathcal{A}}, j \notin \mathcal{S}^*\}$. Eq. (3.2b) is derived by setting $J^* = \bar{\mathcal{A}}/\mathcal{S}^*$ in Eq. (2.4). The initial condition of $DAE(\bar{\mathcal{A}}/\mathcal{S}^*)$ refers to the non-regular KKT point, $x(\tilde{t}) = \bar{x}$, $v(\tilde{t}) = v^*$, $\lambda(\tilde{t}) = \lambda^*$ and $\mu(\tilde{t}) = \mu^*$.

We assume that

$$\nabla_v h_i(\bar{x}, v^*),\ i \in I,\ \nabla_v l_j(\bar{x}, v^*),\ j \in \bar{\mathcal{A}}, \text{ are linearly independent (LICQ)}, \tag{3.3a}$$

$$\nabla_v^2 L(\bar{x}, z^*)|_{KerB^T_{\bar{\mathcal{A}}/\mathcal{S}}} \text{ is non-singular.} \tag{3.3b}$$

Lemma 3.2. *If Condition* (3.3) *hold, then* $\forall \mathcal{S}^* \in \Theta$, *Condition* (2.10) *holds for* $J^* = \bar{\mathcal{A}}/\mathcal{S}^*$.

Proof. Because $\bar{\mathcal{A}}/\mathcal{S}^* \subseteq \bar{\mathcal{A}}$, it is straightforward to see that, if we choose $J^* = \bar{\mathcal{A}}/\mathcal{S}^*$, Condition (3.3a) ensures that Condition (2.10a) holds, $\forall \mathcal{S}^* \in \Theta$. Because $\bar{\mathcal{A}}/\mathcal{S} \subseteq \bar{\mathcal{A}}/\mathcal{S}^*$,

$$KerB^T_{\bar{\mathcal{A}}/\mathcal{S}} \supseteq KerB^T_{\bar{\mathcal{A}}/\mathcal{S}^*}.$$

Therefore, Condition (3.3b) ensures Condition (2.10b) for $J^* = \bar{\mathcal{A}}/\mathcal{S}^*$, $\forall \mathcal{S}^* \subseteq \mathcal{S}$. $\square$

An important consequence of Lemma 3.2 is that, $\forall \mathcal{S}^* \in \Theta$, $DAE(\bar{\mathcal{A}}/\mathcal{S}^*)$ is locally index-1. Therefore, $\forall \mathcal{S}^* \in \Theta$, solutions of Eq. (3.2) are well defined. In other words, we find a number of index-1 DAE systems, which are initialized from the non-regular KKT point $x = \bar{x}$, $z = z^*$. We note that, because SC condition is voilated at non-regular points, continued simulation of $DAE(\bar{\mathcal{A}}/\mathcal{S}^*)$ may violate Eqs. (2.5b), (2.5c). Therefore, the trick of solving OCDE from a non-regular point is to properly select a

$\mathcal{S}_0^* \in \Theta$ such that Eqs. (2.5b), (2.5c) are fulfilled for $t > \tilde{t}$. Note also that, if $\mathcal{S} = \emptyset$, i.e. SC condition holds, then Condition (3.3) reduces to Condition (2.14).

To set up the relationship between the solution of Eq. (3.2) and the KKT points, defined in Eq. (2.5), we next prove that, if a proper $\mathcal{S}^*$ is chosen, the solution of index-1 system (3.2) is the solution of OCDE (1.2) starting from a non-regular KKT point.

Lemma 3.3. *$\forall \mathcal{S}^* \in \Theta$, if $(x^T, v^T, \lambda^T, \mu^T)^T$ satisfies Eq.* (3.2b)*, then*

$$\bar{\mathcal{A}}/\mathcal{S}^* \subseteq \mathcal{A}(x, v), \tag{3.4}$$

where $\bar{\mathcal{A}} := \mathcal{A}(\bar{x}, v^*)$ refers to the active set of inequalities at the non-regular point $x = \bar{x}$, $z = z^*$.

Proof. The proof follows directly from the definition of function $F_{\bar{\mathcal{A}}/\mathcal{S}^*}$. That is, Eq. (3.2b) requires that

$$l_j(x, v) = 0, \quad \forall j \in \mathcal{A}(\bar{x}, v^*)/\mathcal{S}^*.$$

□

Corollary 3.4. *$\forall \mathcal{S}^* \in \Theta$, if $(x^T, v^T, \lambda^T, \mu^T)^T$ satisfies Eq.* (3.2b)*, then it satisfies Eq.* (2.5a)*.*

Proof. From the definition of $F_{\mathcal{A}(x,v)}$ in Eq. (2.5a),

$$l_j(x, v) = 0, \quad \forall j \in \mathcal{A}(x, v),$$

hold automatically. Therefore, we only need to prove that

$$\mu_j = 0, \quad \forall j \notin \mathcal{A}(x, v).$$

This equation is true, because

$$u_j = 0, \quad \forall j \notin \bar{\mathcal{A}}/\mathcal{S}^*,$$

which is ensured by Eq. (3.2b), and Eq. (3.4). □

Hence, from the definition (3.2) of system $DAE(\bar{\mathcal{A}}/\mathcal{S}^*)$, the solutions of $DAE(\bar{\mathcal{A}}/\mathcal{S}^*)$ always satisfy the "equality" part of the KKT conditions, namely Eq. (2.5a). The "inequality" part, namely Eqs. (2.5b)–(2.5c), may get violated, however, because of the damage of SC condition. A reasonable way to continue simulation from the non-regular KKT point $x = \bar{x}$, $z = z^*$ at $t = \tilde{t}$ is to choose a $\mathcal{S}_0^* \in \Theta$ such that the solution of $DAE(\bar{\mathcal{A}}/\mathcal{S}_0^*)$ fulfills Eqs. (2.5b)–(2.5c) also.

More exactly, consider that the non-regular KKT point $x = \bar{x}$, $z = z^*$ at $t = \tilde{t}$. For each $\mathcal{S}^* \in \Theta$, denote $x^{\mathcal{S}^*}(t)$, $z^{\mathcal{S}^*}(t) = (v^{\mathcal{S}^*}(t)^T, \lambda^{\mathcal{S}^*}(t)^T, \mu^{\mathcal{S}^*}(t)^T)^T$ as the solution of index-1 $DAE(\bar{\mathcal{A}}/\mathcal{S}^*)$ starting from $t = \tilde{t}$. From Corollary 3.4, we know that $x^{\mathcal{S}^*}(t)$, $z^{\mathcal{S}^*}(t)$ always satisfy Eq. (2.5a) (Eqs. (2.5b)–(2.5c) may get violated). Assume that there exists a $\mathcal{S}_0^* \in \Theta$ (The choice may not be unique!) such that inequality constraints (2.5b)–(2.5c), i.e.

$$
\begin{aligned}
l_j(x^{\mathcal{S}_0^*}(t), v^{\mathcal{S}_0^*}(t)) &\geq 0, \quad j \in J, \\
\mu_j^{\mathcal{S}_0^*}(t) &\geq 0, \quad j \in J,
\end{aligned} \tag{3.5}
$$

hold for $t \in [\tilde{t}, \tilde{t}+\epsilon]$. $\epsilon > 0$ denotes an arbitrarily small number. $x^{\mathcal{S}_0^*}(t)$, $z^{\mathcal{S}_0^*}(t)$ refer to the solution of $DAE(\bar{\mathcal{A}}/\mathcal{S}_0^*)$ starting from the non-regular KKT point at $t = \tilde{t}$.

Eq. (3.5) can be ensured by imposing the so-called transversality condition

$$
\begin{aligned}
\frac{dl_j(x^{\mathcal{S}_0^*}(t), v^{\mathcal{S}_0^*}(t))}{dt}\Big|_{t=\tilde{t}} &> 0, \quad \forall j \in \mathcal{S}_0^*, \\
\frac{d\mu_j^{\mathcal{S}_0^*}(t)}{dt}\Big|_{t=\tilde{t}} &> 0, \quad \forall j \in \mathcal{S}/\mathcal{S}_0^*.
\end{aligned} \tag{3.6}
$$

Eq. (3.6) is a sufficient condition of Eq. (3.5). It guarantees that SC condition is only violated at $t = \tilde{t}$. This is proved in the following lemma.

Lemma 3.5. *If Eq.* (3.6) *holds at $t = \tilde{t}$, then:* (1) *There exists $\epsilon > 0$ such that Eq.* (3.5) *holds for $t \in [\tilde{t}, \tilde{t}+\epsilon]$.* (2) *$\forall t \in (\tilde{t}, \tilde{t}+\epsilon]$, SC condition holds, i.e. SC condition is violated only at $t = \tilde{t}$.*

Proof. From the definitions of J, $\bar{\mathcal{A}}$, $\mathcal{S}$ and $\mathcal{S}_0^*$ introduced above, we have $\mathcal{S}_0^* \subseteq \mathcal{S} \subseteq \bar{\mathcal{A}} \subseteq J$. Therefore,

$$0 = \mu_j^{\mathcal{S}_0^*}(\tilde{t}), \qquad l_j(x^{\mathcal{S}_0^*}(\tilde{t}), v^{\mathcal{S}_0^*}(\tilde{t})) > 0, \qquad j \in J/\bar{\mathcal{A}}, \tag{3.7a}$$

$$0 = l_j(x^{\mathcal{S}_0^*}(\tilde{t}), v^{\mathcal{S}_0^*}(\tilde{t})), \qquad \mu_j^{\mathcal{S}_0^*}(\tilde{t}) > 0, \qquad j \in \bar{\mathcal{A}}/\mathcal{S}, \tag{3.7b}$$

$$0 = l_j(x^{\mathcal{S}_0^*}(\tilde{t}), v^{\mathcal{S}_0^*}(\tilde{t})), \qquad \mu_j^{\mathcal{S}_0^*}(\tilde{t}) = 0, \qquad j \in \mathcal{S}/\mathcal{S}_0^*, \tag{3.7c}$$

$$0 = \mu_j^{\mathcal{S}_0^*}(\tilde{t}), \qquad l_j(x^{\mathcal{S}_0^*}(\tilde{t}), v^{\mathcal{S}_0^*}(\tilde{t})) = 0, \qquad j \in \mathcal{S}_0^*. \tag{3.7d}$$

The first terms in Eqs. (3.7a)–(3.7d) correspond to Eq. (3.2b). Points (1) (2) follow by applying Eq. (3.6) to the second terms in Eqs. (3.7c)–(3.7d). □

Note that, Condition (3.6) is called transversality condition, because $l_j(x^{\mathcal{S}_0^*}(t), v^{\mathcal{S}_0^*}(t))$, $j \in \mathcal{S}_0^*$, and $\mu_j^{\mathcal{S}_0^*}(t)$, $j \in \mathcal{S}/\mathcal{S}_0^*$, change the signs around $t = \tilde{t}$. Note also that, Eq. (3.6) can be evaluated numerically by applying the chain rule to Eq. (3.2b).

To summarize the discussion above,

Theorem 3.6. *Denote $(\bar{x}^T, z^{*T})^T$ as a non-regular KKT point where SC condition fails for $t = \tilde{t}$, if Condition* (3.3) *holds and if there exists a $\mathcal{S}_0^* \in \Theta$ such that the transversality condition* (3.6) *holds, then:* (1) *$DAE(\bar{\mathcal{A}}/\mathcal{S}_0^*)$, starting from $x(\tilde{t}) = \bar{x}$ and $z(\tilde{t}) = z^*$, is locally of index* 1. (2) *There exists $\epsilon > 0$, such that solutions $x^{\mathcal{S}_0^*}(t)$, $z^{\mathcal{S}_0^*}(t)$ of $DAE(\bar{\mathcal{A}}/\mathcal{S}_0^*)$ correspond to the KKT points of $P(x^{\mathcal{S}_0^*}(t))$ for $t \in [\tilde{t}, \tilde{t}+\epsilon)$.* (3) *Along the solution trajectory $x^{\mathcal{S}_0^*}(t)$, $z^{\mathcal{S}_0^*}(t)$, $t \in [\tilde{t}, \tilde{t}+\epsilon)$, SC condition is violated only at $t = \tilde{t}$.*

Theorem 3.6 says that to solve OCDE starting from a non-regular KKT point (where SC condition fails) one can solve DAE system (3.2) with a properly selected index set $\mathcal{S}_0^*$. Sufficient conditions are given such that the derived DAE system (3.2) is of index-1 and its solution satisfies KKT condition (2.5). The proposed transversality condition (3.6) makes sure that SC condition is violated only at $t = \tilde{t}$, and therefore, for $t \in (\tilde{t}, \tilde{t}+\epsilon]$, $z^{\mathcal{S}_0^*}(t)$ refers to regular KKT points of $P(x^{\mathcal{S}_0^*}(t))$.

The switching behavior can be now explained. Consider at $t = \tilde{t}_- < \tilde{t}$, $x(\tilde{t}_-)$ and $v(\tilde{t}_-)$ correspond to a regular KKT point. Denote $\bar{\mathcal{A}}'$ as the active set of $P(x(\tilde{t}_-))$ at $t = \tilde{t}_-$, i.e.

$$\bar{\mathcal{A}}' = \mathcal{A}(x(\tilde{t}_-), v(\tilde{t}_-)). \tag{3.8}$$

From Section 3.1, near this regular point we solve $DAE(\bar{\mathcal{A}}')$. Denote $x^{\bar{\mathcal{A}}'}(t)$, $z^{\bar{\mathcal{A}}'}(t)$ as the solution of $DAE(\bar{\mathcal{A}}')$. Assume that the solution of $DAE(\bar{\mathcal{A}}')$ can extend from $t = \tilde{t}_-$ to $t = \tilde{t}$, where SC condition is damage at $t = \tilde{t}$. Denote

$$\bar{\mathcal{A}} = \mathcal{A}(x^{\bar{\mathcal{A}}'}(\tilde{t}), v^{\bar{\mathcal{A}}'}(\tilde{t})) \tag{3.9}$$

as the active set of $P(x^{\bar{\mathcal{A}}'}(\tilde{t}))$ at $t = \tilde{t}$. We note that $\bar{\mathcal{A}}' \subseteq \bar{\mathcal{A}}$ (If at least an inequality constraint is activated at $t = \tilde{t}$, $\bar{\mathcal{A}}' \subset \bar{\mathcal{A}}$. Otherwise, when some positive Lagrangian multipliers of active inequality constraints at $t = \tilde{t}_-$ become zeros at $t = \tilde{t}$, $\bar{\mathcal{A}}' = \bar{\mathcal{A}}$.). Denote $\mathcal{S}'$ as the index set of active inequality constraints at $t = \tilde{t}$, for which SC condition fails. That is,

$$\mathcal{S}' := \{j \in J \mid j \in \bar{\mathcal{A}},\ \mu_j^{\bar{\mathcal{A}}'}(\tilde{t}) = 0\} \neq \emptyset.$$

At $t = \tilde{t}$, the following lemma gives sufficient conditions such that the solutions $x^{\bar{\mathcal{A}}'}(t)$, $z^{\bar{\mathcal{A}}'}(t)$ of $DAE(\bar{\mathcal{A}}')$ violate inequality constraints (2.5b)–(2.5c) for $t = \tilde{t}^+ > \tilde{t}$.

Lemma 3.7. *(i) If $\exists\, j^* \in \mathcal{S}'/\bar{\mathcal{A}}'$ such that*

$$\frac{dl_{j^*}(x^{\bar{\mathcal{A}}'}(t), v^{\bar{\mathcal{A}}'}(t))}{dt}\Big|_{t=\tilde{t}} < 0, \tag{3.10}$$

then $l_{j^*}(x^{\bar{\mathcal{A}}'}(t), v^{\bar{\mathcal{A}}'}(t))$ changes its sign from positive to negative around $t = \tilde{t}$, which violates Eq. (2.5b)*.*

(ii) If $\exists\, j^* \in \bar{\mathcal{A}}' \cap \mathcal{S}'$ such that

$$\frac{d\mu_{j^*}^{\bar{\mathcal{A}}'}(t)}{dt}\Big|_{t=\tilde{t}} < 0, \tag{3.11}$$

then $\mu_{j^*}^{\bar{\mathcal{A}}'}(t)$ changes its sign from positive to negative around $t = \tilde{t}$, which violates Eq. (2.5c)*.*

Proof. (i) For $j^* \notin \bar{\mathcal{A}}'$, we have $l_{j^*}(x^{\bar{\mathcal{A}}'}(t), v^{\bar{\mathcal{A}}'}(t)) > 0$, at $t = \tilde{t}_- < \tilde{t}$. For $j^* \in \mathcal{S}'$, we have $l_{j^*}(x^{\bar{\mathcal{A}}'}(t), v^{\bar{\mathcal{A}}'}(t)) = 0$ at $t = \tilde{t}$. Therefore, for $j^* \in \mathcal{S}'/\bar{\mathcal{A}}'$, Eq. (3.10) ensures that $l_{j^*}(x^{\bar{\mathcal{A}}'}(t), v^{\bar{\mathcal{A}}'}(t))$ changes its sign from positive to negative around $t = \tilde{t}$. (ii) For

$j^* \in \bar{\mathcal{A}}'$, we have $\mu_{j^*}^{\bar{\mathcal{A}}'}(t) > 0$ at $t = \tilde{t}_- < \tilde{t}$. For $j^* \in \mathcal{S}'$, we have $\mu_{j^*}^{\bar{\mathcal{A}}'}(t) = 0$ at $t = \tilde{t}$. Therefore, for $j^* \in \bar{\mathcal{A}}' \cap \mathcal{S}'$, we have $\mu_{j^*}^{\bar{\mathcal{A}}'}(t)$ changes its sign from positive to negative around $t = \tilde{t}$. □

Eqs. (3.10), (3.11) are also called transversality conditions, which are analogous to Eq. (3.6). These conditions ensure that the solutions of $DAE(\bar{\mathcal{A}}')$, $x^{\bar{\mathcal{A}}'}(t)$, $z^{\bar{\mathcal{A}}'}(t)$ do not satisfy the feasibility conditions (2.5b)–(2.5c) for $t > \tilde{t}$.

Hence, at $t = \tilde{t}$ (the non-regular point) one has to construct a new DAE system, denoted as $DAE(\bar{\mathcal{A}}/\mathcal{S}_0^*)$, and solve $DAE(\bar{\mathcal{A}}/\mathcal{S}_0^*)$ initialized from $x(\tilde{t}) = x^{\bar{\mathcal{A}}'}(\tilde{t})$ and $z(\tilde{t}) = z^{\bar{\mathcal{A}}'}(\tilde{t})$. Because $\bar{\mathcal{A}}' \neq \bar{\mathcal{A}}/\mathcal{S}_0^*$, $DAE(\bar{\mathcal{A}}')$ and $DAE(\bar{\mathcal{A}}/\mathcal{S}_0^*)$ are defined differently. The structural change of solved DAE systems before and after $t = \tilde{t}$ leads to the switching behavior of OCDE.

At the end, we note that it is assumed that $\mathcal{S}_0^*$ exists. In case that such $\mathcal{S}_0^*$ does not exist, NLP solvers may be applied to find another local minimizers v^{**}, $v^{**} \neq v^*$, of $P(\bar{x})$ and start simulation from there. In this case, jumps of variables v along the solution trajectory will appear. Note also that, there may exist not only one $\mathcal{S}_0^* \in \Theta$ such that Eq. (3.6) is fulfilled. This situation seems to happen more frequently, when $\mathcal{S}$ contains multiple elements. If thsi is the case, depending on the selection of $\mathcal{S}_0^*$, the solution of OCDE may not be unique.

3.3. **A solution algorithm.** From the discussion above, to solve OCDE (1.2) at regular points one can directly apply classical DAE solvers to Eq. (3.1). If non-regular points (SC condition is damaged) are encountered at time $t = \tilde{t}$, one reconstructs a new DAE system (3.2) with a properly selected $\mathcal{S}_0^*$ and restart the simulation from there. This composes the major steps of solving OCDE.

To locate the switching points where SC condition is damaged, we propose the following event function

$$\phi_j(t) := l_j(x(t), v(t)) - \mu_j(t), \quad \forall j \in J. \tag{3.12}$$

$\phi_j(t)$, $j \in J$, should be monitored along the solution trajectory for locating the switching time $\tilde{t}$. Note that, if Eq. (3.10) or Eq. (3.11) hold, then $\exists\, j \in J$ such that $\phi_j(t)$ changes the sign at $t = \tilde{t}$. If $\phi_j(t)$ changes the sign from negative to positive, it indicates that a further simulation would violate Eq. (2.5c). If $\phi_j(t)$ changes the sign from positive to negative, it indicates that a further simulation would violate Eq. (2.5b), refer to Lemma 3.7. We note also that, methods of locating events (i.e. finding out where the event function exactly changes the sign) for DAE systems are already proposed in the literature. We refer to e.g. [20, 3] and the reference therein for this issue.

Solution Algorithm:

1. Initialize: At $t = 0$, $x(0) = x_0$, solve $P(x_0)$ by NLP solvers. Denote the optimal solution as $z_0 = (v_0^T, \lambda_0^T, \mu_0^T)^T$. If z_0 is not a regular KKT point, set $\tilde{t} = 0$, go to step 3. Otherwise set $\bar{\mathcal{A}} = \mathcal{A}(x_0, v_0)$, $\mathcal{S}_0^* = \emptyset$, $t_{start} = 0$, $x_{start} = x_0$, $z_{start} = z_0$.
2. Major integration: Solve $DAE(\bar{\mathcal{A}}/\mathcal{S}_0^*)$, defined in Eq. (3.2) with initial condition $x(t_{start}) = x_{start}$ and initial guess $z(t_{start}) = z_{start}$. Stop simulation until either $t = t_{end}$ (in this case, stop and quit) or SC condition is violated at $t = \tilde{t}$ by checking the event function (3.12). Go to step 3.
3. Switching: Set $\bar{\mathcal{A}} = \mathcal{A}(x(\tilde{t}), v(\tilde{t}))$. Select a $\mathcal{S}_0^* \in \Theta$ such Eq. (3.6) holds for $DAE(\bar{\mathcal{A}}/\mathcal{S}_0^*)$. Set $t_{start} = \tilde{t}$, $x_{start} = x(\tilde{t})$, $z_{start} = z(\tilde{t})$. Go to step 2.

Note that the initial guess of variable z, denoted as z_{start}, is to avoid starting simulation from other local minimizers. Note also that in Step 3, if no $\mathcal{S}_0^*$ can be found, one can use NLP solvers to solve $P(x_{start})$ for another local minimizer z' and start simulation from $z = z'$. In this case, jumps of variables $z(t)$ will appear at $t = \tilde{t}$.

At the end, we need to note that, the proposed algorithm is limited to case that conditions in Theorem 3.6, i.e. Conditions (3.3), (3.6) and the existence of $\mathcal{S}_0^*$, hold. When any of them are violated, one may encounter numerical difficulties. This remains interesting questions to be investigated in the further.

4. EXAMPLES

4.1. **A mathematical example.** We consider to solve the following example:

$$\dot{y_1} = 0.5 + x_1 x_2, y_1(0) = \pi/4, \tag{4.1a}$$

$$\dot{y_2} = y_1, y_2(0) = 0, \tag{4.1b}$$

$$(x_1, x_2) \in \text{argmin}_{x_1,x_2}\ x_1^2 + x_2^2, \tag{4.1c}$$

$$s.t.\ 1.7\sin(y_1) + x_2 - e^{-x_1} \geq 0, \tag{4.1d}$$

$$0.2\cos(y_2) + 2 - x_2 \geq 0. \tag{4.1e}$$

y_1, y_2, x_1, $x_2 \in \mathbb{R}$. $y = (y_1, y_2)^T$ refer to the states of the dynamic system. $x = (x_1, x_2)^T$ refer to the optimization variables of the inner optimization problem $P(y)$, defined by Eqs. (4.1c)–(4.1e). We use $l_j(\cdot) \geq 0$, $j = 1, 2$, to refer to the inequality constraints (4.1d) and (4.1e), respectively. μ_j, $j = 1, 2$, refer to their Lagrangian multipliers. $\phi_j := l_j - \mu_j$, $j = 1, 2$, are derived event functions, refer to Eq. (3.12).

By applying the proposed solution algorithm, Fig. 1 to Fig. 4 show the computational results of solving OCDE (4.1) for $t \in [0, 20]$. Fig. 1 shows the optimal solution $x(t)$ of the inner optimization problem $P(y(t))$ for $t \geq 0$. Fig. 2 shows the values of inequality constraints $l_1(\cdot)$ and $l_2(\cdot)$, namely Eqs. (4.1d), (4.1e), along the solution curve. It can be seen that the inequality constraints are always fulfilled for $t \geq 0$. Fig. 3 shows the values of Lagrangian multipliers μ_1 and μ_2 for $t \geq 0$. As we can see from the figure, μ_1 and μ_2 fulfill Eq. (2.5c) always. Fig. 4 shows the values of

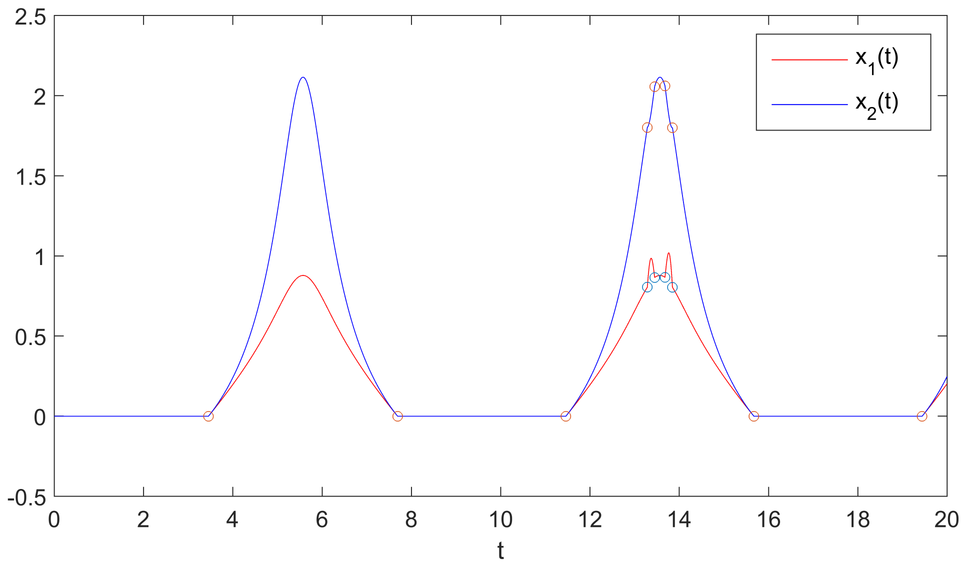

FIGURE 1. Simulation results of $x_1(t)$ and $x_2(t)$, $t \in [0, 20]$.

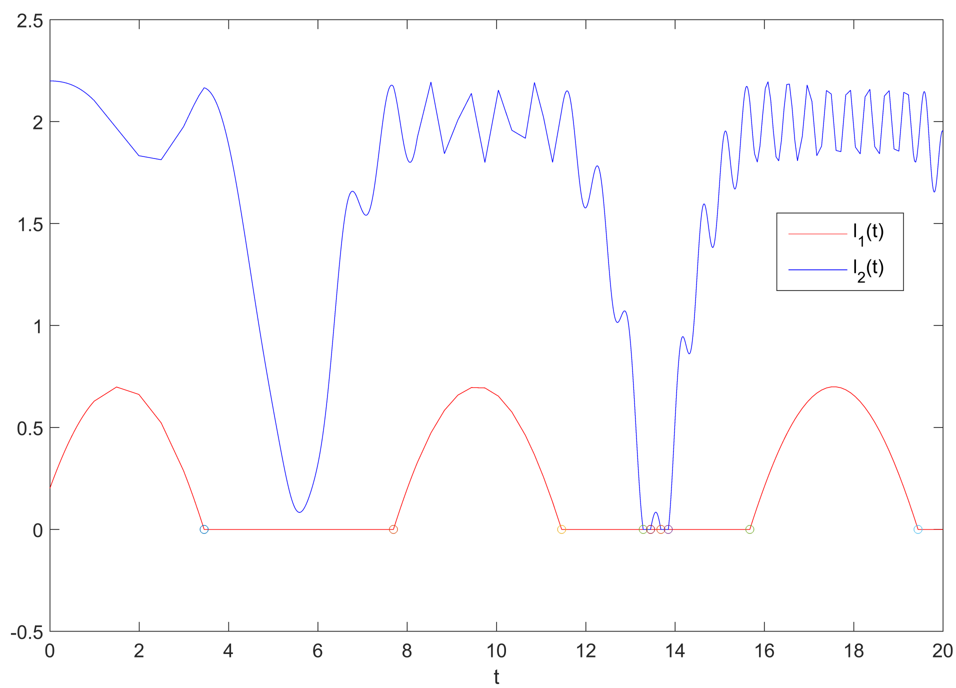

FIGURE 2. Simulation results of inequality constraints $l_1(t)$ and $l_2(t)$, $t \in [0, 20]$.

event functions $\phi_j(t)$, $j = 1, 2$, defined in Eq. (3.12). When ϕ_j changes its sign from positive to negative, it indicates that the inequality constraint $l_j(\cdot) \geq 0$ is activated. When ϕ_j changes its sign from negative to positive, it indicates that the inequality

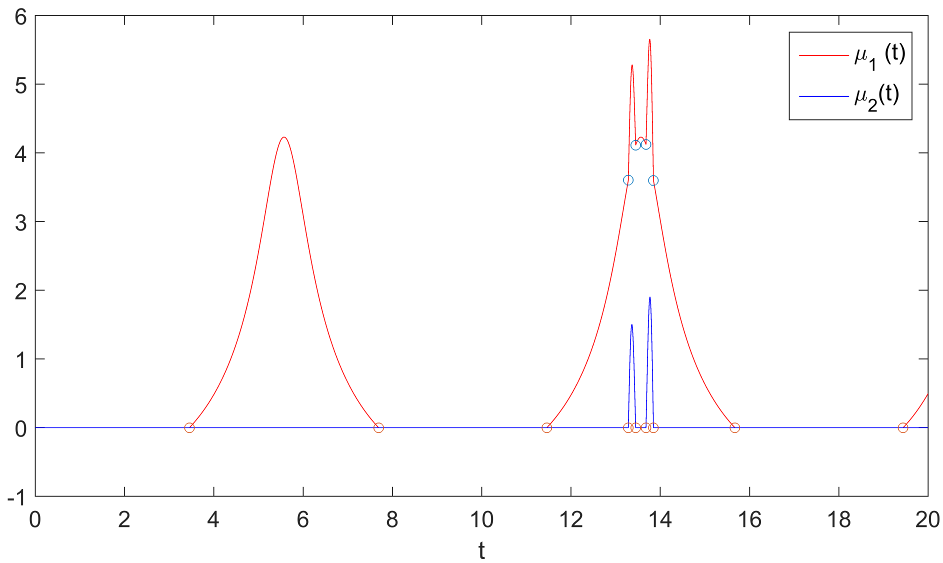

FIGURE 3. Simulation results of Lagrangian multipliers $\mu_1(t)$ and $\mu_2(t)$, $t \in [0, 20]$.

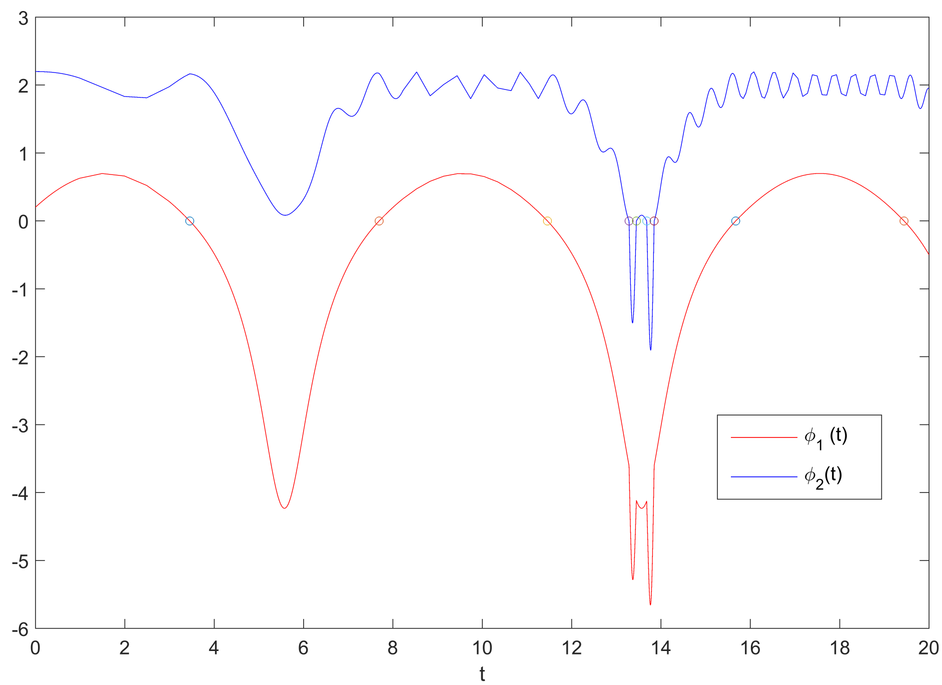

FIGURE 4. Simulation results of the event functions $\phi_1(t)$ and $\phi_2(t)$, $t \in [0, 20]$.

constraint $l_j(\cdot) \geq 0$ is deactivated. Cycles in Fig. 1 to Fig. 4 refer to the switching time of OCDE.

Table 1 lists the computed switching time $\tilde{t}_k$, $k = 1, \ldots, 9$, the active set $\bar{\mathcal{A}} = \mathcal{A}(y(\tilde{t}_k), x(\tilde{t}_k))$, the index set $\mathcal{S}$ of inequality constraints, for which the SC condition

TABLE 1. $\tilde{t}_k$, $k = 1, \ldots, 9$, refer to the switching time during the solution curve of OCDE (4.1) for $t \in [0, 20]$. For each switching time $\tilde{t}_k$, $\bar{\mathcal{A}} = \mathcal{A}(y(\tilde{t}_k), x(\tilde{t}_k))$ refers to the active set of the inner optimization problem $P(y(t))$ at $t = \tilde{t}_k$. Set $\mathcal{S}$ refers to the index of inequality constraints, for which SC condition is damaged at $t = \tilde{t}_d$. $\mathcal{S}_0^*$ refers to a selected subset of $\mathcal{S}$, such that $DAE(\bar{\mathcal{A}}/\mathcal{S}_0^*)$ is solved for $\tilde{t}_k \le t \le \tilde{t}_{k+1}$. The solution of $DAE(\bar{\mathcal{A}}/\mathcal{S}_0^*)$ corresponds to the solution of the original OCDE for the time period $[\tilde{t}_k, \tilde{t}_{k+1}]$.

$\tilde{t}_k$	$\bar{\mathcal{A}}$	$\mathcal{S}$	$\mathcal{S}_0^*$	$\bar{\mathcal{A}}/\mathcal{S}_0^*$
3.4546	$\{1\}$	$\{1\}$	$\emptyset$	$\{1\}$
7.6931	$\{1\}$	$\{1\}$	$\{1\}$	$\emptyset$
11.4608	$\{1\}$	$\{1\}$	$\emptyset$	$\{1\}$
13.2868	$\{1,2\}$	$\{2\}$	$\emptyset$	$\{1,2\}$
13.4506	$\{1,2\}$	$\{2\}$	$\{2\}$	$\{1\}$
13.6819	$\{1,2\}$	$\{2\}$	$\emptyset$	$\{1,2\}$
13.8492	$\{1,2\}$	$\{2\}$	$\{2\}$	$\{1\}$
15.6742	$\{1\}$	$\{1\}$	$\{1\}$	$\emptyset$
19.4419	$\{1\}$	$\{1\}$	$\emptyset$	$\{1\}$

is violated, the selected subset $\mathcal{S}_0^*$ of $\mathcal{S}$ and the index set $\bar{\mathcal{A}}/\mathcal{S}_0^*$ for constructing DAE system $DAE(\bar{\mathcal{A}}/\mathcal{S}_0^*)$. We note that $DAE(\bar{\mathcal{A}}/\mathcal{S}_0^*)$ is used to solve OCDE for the time period $[\tilde{t}_k, \tilde{t}_{k+1}]$. At the starting time $t = 0$ and the end time $t = 20$, the inner optimization problems $P(y(0))$ and $P(y(20))$ have regular KKT points.

To illustrate the proposed algorithm, let us look at the first and second switches at $\tilde{t}_1 = 3.4546$ and $\tilde{t}_2 = 7.6931$. At initial time ($t = 0$), the active set $\mathcal{A}(y(0), x(0))$ of $P(y(0))$ is empty and the optimal solution of $P(y(0))$ corresponds to a regular KKT point. Therefore for $t \in [0, \tilde{t}_1]$ we solve $DAE(\mathcal{A}(y(0), x(0))) = DAE(\emptyset)$. At $t = \tilde{t}_1$, the event function $\phi_1(t)$ changes its sign from positive to negative, refer to Fig. 4. This indicates that a continued simulation of $DAE(\mathcal{A}(y(0), x(0)))$ will violate inequality constraint (4.1d). At $t = \tilde{t}_1$, $\mathcal{A}(y(\tilde{t}_1), x(\tilde{t}_1)) = \{1\}$, refer to Table 1, and if we choose $\mathcal{S}_0^* = \emptyset$, the resulted $DAE(\bar{\mathcal{A}}/\mathcal{S}_0^*) = DAE(\{1\})$ satisfies transversality condition (3.6). So for $t \in [\tilde{t}_1, \tilde{t}_2]$, we solve $DAE(\{1\})$ starting from $y(\tilde{t}_1)$ and $x(\tilde{t}_1)$. The switching behavior of OCDE at $t = \tilde{t}_1$ is caused by activating the first inequality constraint (4.1d).

At $t = \tilde{t}_2$, the event function $\phi_1(t)$ changes its sign from negative to positive, refer to Fig. 4. This indicates that a continued simulation will violate $\mu_1 \ge 0$ (which is imposed by the KKT condition (2.5c)). At this time point, $\bar{\mathcal{A}} = \mathcal{A}(y(\tilde{t}_2), x(\tilde{t}_2)) = \{1\}$ and if we choose $\mathcal{S}_0^* = \{1\}$, the resulted $DAE(\bar{\mathcal{A}}/\mathcal{S}_0^*) = DAE(\emptyset)$ satisfies the

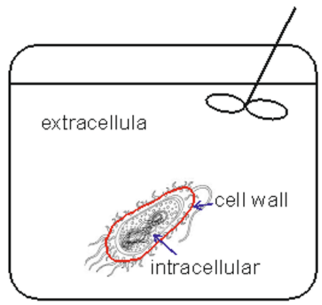

FIGURE 5. Bioreactor.

transversality condition (3.6) at $\tilde{t}_2$. So for $t \in [\tilde{t}_2, \tilde{t}_3]$, we solve $DAE(\emptyset)$ starting from $y(\tilde{t}_2)$ and $x(\tilde{t}_2)$.

As we can see from the previous discussion, for $t \in [0, \tilde{t}_1]$ we solve $DAE(\emptyset)$, for $t \in [\tilde{t}_1, \tilde{t}_2]$ we solve $DAE(\{1\})$, and for $t \in [\tilde{t}_2, \tilde{t}_3]$ we solve $DAE(\emptyset)$. Switching behavior is therefore expected at $\tilde{t}_1$ and $\tilde{t}_2$, because different DAE systems are solved sequentially. This procedure is repeated analogously until the end time $t = 20$ is reached.

4.2. **Simulation of bioreactors.** In this section, we present an OCDE example from systems biotechnology and apply the presented solution algorithm to solve it. Consider a fermentation process, which takes place in a continuous stirred-tank reactor, shown in Fig. 5. A microorganism is placed inside the reactor, which transforms substrate A to products F. Denote $X \in \mathbb{R}$ in $[g_{BM}/L]$ as the concentration of the microorganism in the fluid medium. Denote $S, P \in \mathbb{R}$ in $[mmol/L]$ as the concentrations of substrate A and product F in the fluid medium, respectively.

Fig. 6 shows a simplified metabolic network of the studied microorganism [21]. Rectangles represent metabolites, which are either intracellular (A, B, $\ldots$, F) or extracellular (A_{ex}, E_{ex} and F_{ex}). Diamonds represent reactions. The reaction rates in $[mmol/g_{BM}/h]$ are denoted as $v_{upt}, v_1, \ldots, v_7$, respectively. "upt" is short for uptake. One-direction arrows mean that the corresponding reactions are irreversible, while two-direction arrows represent reversible reactions. Note that, metabolites A_{ex} and F_{ex} refer to extracellular substrate and product, respectively. E_{ex} represents a metabolite which contributes to the growth of microorganism.

The mass balances of the fluid medium can be modeled by

$$\dot{X} = v_6 X, X(0) = 1, \tag{4.2a}$$

$$\dot{S} = -v_{upt} X, S(0) = 20, \tag{4.2b}$$

$$\dot{P} = v_7 X, P(0) = 0. \tag{4.2c}$$

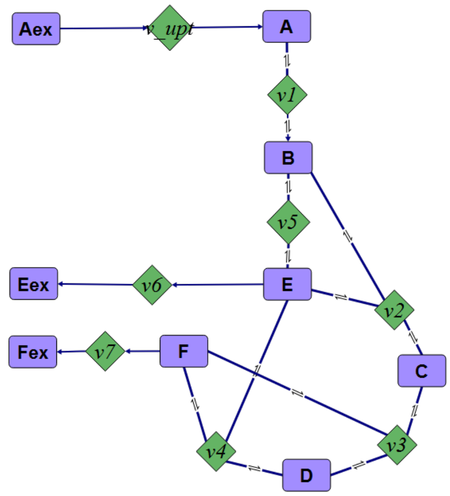

FIGURE 6. Simplified metabolic network of studied microorganism.

In order to formulate the inner optimization problem, we define

$$d(t) = \frac{1}{a\sqrt{\pi}} e^{\frac{-(t-t_s)^2}{a^2}}$$

as an approximated impulse function with trigger time $t_s = 0.5$. $a > 0$ is chosen sufficiently small (in our example $a = 0.02$). Approximated step function $\alpha(t)$ can be therefore generated by integrating

$$\dot{\alpha} = d(t), \quad \alpha(0) = 0, \tag{4.3a}$$

$$\dot{t} = 1, \quad t(0) = 0, \tag{4.3b}$$

where derivatives of time t is explicitly given in Eq. (4.3b)[1]. $\alpha(t)$ takes the value of 0 at $t = 0$ and jumps to the value of 1 near the trigger time $t = t_s$. $\alpha(t)$ will be used later to formulate the inner optimization problem. Now if we consider $(X, S, P, \alpha, t)^T$ as variables x in Eq. (1.2a), Eqs. (4.2), (4.3) form the upper level part of OCDE (1.2).

To define the inner optimization problem, denote vector $v = (v_{upt}, v_1, ..., v_7)^T \in \mathbb{R}^8$. In Eq. (4.2), variables v_6, v_7 and v_{upt} have to be determined from solving the following optimization problem.

$$\max_{v} \ \phi(v, \alpha) \tag{4.4a}$$

$$s.t. Mv = 0, \tag{4.4b}$$

$$v_{upt} = \frac{v_m S}{S + K_{upt}}, \tag{4.4c}$$

$$v_6 \geq 0, \tag{4.4d}$$

$$v_7 \geq 0, \tag{4.4e}$$

[1]Because we want to bring the obtained OCDE example (4.2), (4.3) and (4.4) in line with the standard OCDE formulation (1.2).

with $v_m = 3.8$, $K_{upt} = 1$,

$$\phi(v, \alpha) := (1-\alpha)\frac{v_6}{\sqrt{v^T v}} + \alpha \frac{v_7}{\sqrt{v^T v}} \tag{4.5}$$

and

$$M = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

We note that problem (4.4) refers to the Flux Balance Analysis (FBA) [16]. The objective function in Eq. (4.4a) is composed of two parts. Term $v_6/\sqrt{v^T v}$ refers to the growth rate of microorganism, while term $v_7/\sqrt{v^T v}$ refers to the formation rate of product. Since $\alpha(t)$ is an approximated step function, the objective function (4.4a) firstly maximizes the growth rate of microorganism and then maximizes the formation rate of product F.

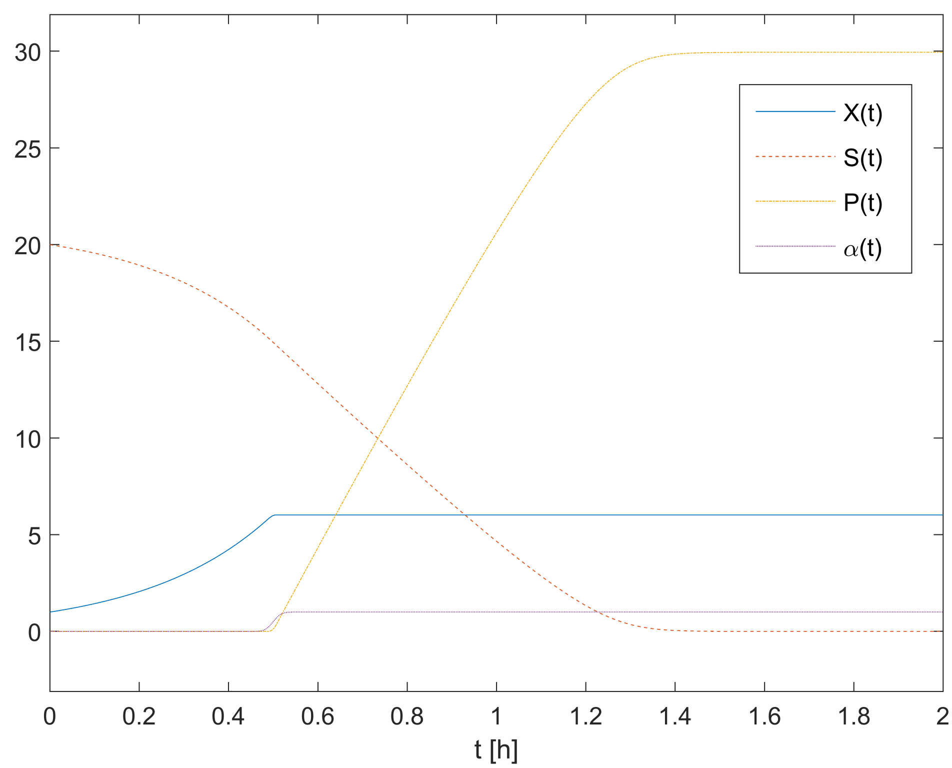

FIGURE 7. Simulation results: States $X(t)$, $S(t)$, $P(t)$ and $\alpha(t)$.

Simulation results of the defined OCDE in Eqs. (4.2), (4.3) and (4.4) are presented in Fig. 7 to Fig. 10. Along the solution trajectories there are in total two switches.

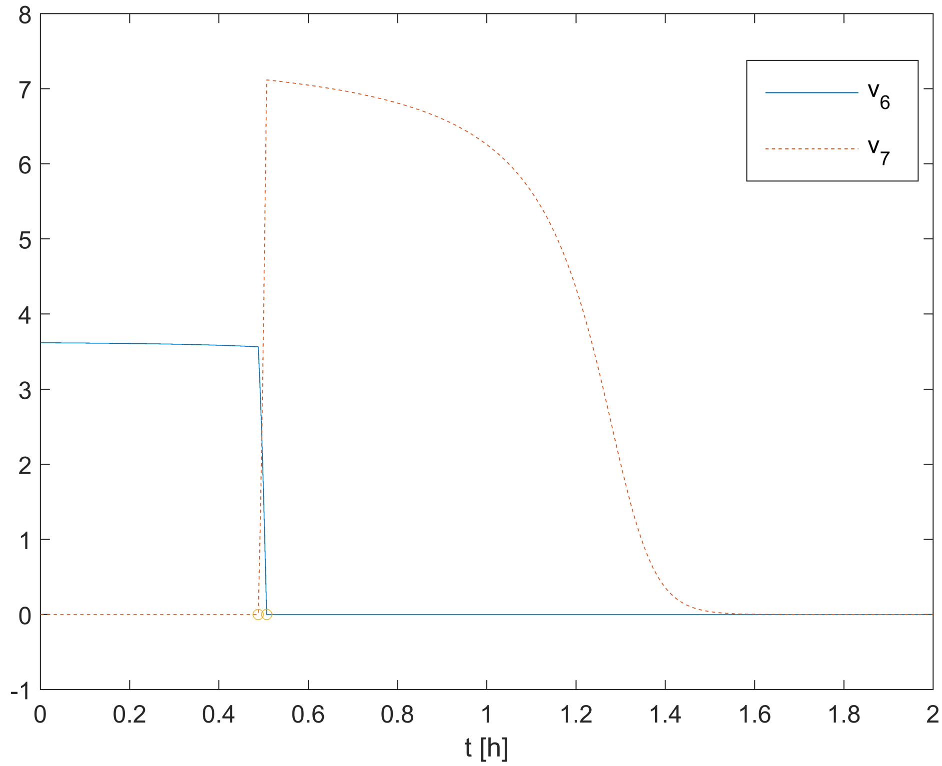

FIGURE 8. Simulation results: $v_6(t)$ and $v_7(t)$ in the inner optimization. Cycles refer to switching times.

TABLE 2. $\tilde{t}_k$, $k = 1, 2$, refer to the switching time during the solution curve of the bioreactor example. For each switching time $\tilde{t}_k$, $\bar{\mathcal{A}} = \mathcal{A}(\tilde{t}_k)$ refers to the active set of the inner optimization problem (4.4) at $t = \tilde{t}_k$. Set $\mathcal{S}$ refers to the index of inequality constraints, for which SC condition is damaged at $t = \tilde{t}_k$. $\mathcal{S}_0^*$ refers to a selected subset of $\mathcal{S}$, such that $DAE(\bar{\mathcal{A}}/\mathcal{S}_0^*)$ is solved for $\tilde{t}_k \le t \le \tilde{t}_{k+1}$.

$\tilde{t}_k$	$\bar{\mathcal{A}}$	$\mathcal{S}$	$\mathcal{S}_0^*$	$\bar{\mathcal{A}}/\mathcal{S}_0^*$
0.4881	$\{2\}$	$\{2\}$	$\{2\}$	$\emptyset$
0.5071	$\{1\}$	$\{1\}$	$\emptyset$	$\{1\}$

One switch happens at $\tilde{t}_1 = 0.4881$ and the other $\tilde{t}_2 = 0.5071$, refer to Table 2. Fig. 7 presents the trajectories of the states of the computed OCDE example. Fig. 8 presents the values of inequality constraints (4.4d), (4.4e), which are kept non-negative along the solution trajectory. Fig. 9 presents the values of Lagrangian multiples for inequality constraints (4.4d), (4.4e), which are hold non-negative. Fig. 10 presents the values of event functions, which change their signs along the solution trajectory. Cycles refer to switching times.

We use $l_j \geq 0$, $j = 1, 2$, to refer to the inequality constraints (4.4d) and (4.4e), respectively. At initial time point $t = 0$, the active set $\mathcal{A}(t = 0) = \{2\}$, $\mathcal{S} = \emptyset$ (SC condition holds) and this point corresponds to a regular KKT point. For $t \in [0, \tilde{t}_1]$ we solve the derived system (3.1), denoted as $DAE(\{2\})$. At $t = \tilde{t}_1$, the event function $\phi_2(t)$ defined in Eq. (3.12) changes its sign from negative to positive, which indicates that a continued simulation will violate inequalities $\mu_2 \geq 0$ imposed by Eq. (2.5c), refer to Fig. 9 and Fig. 10. At $t = \tilde{t}_1$, $\mathcal{A}(\tilde{t}_1) = \{2\}$, $\mathcal{S} = \{2\}$, and if we select $\mathcal{S}_0^* = \{2\} \subseteq \mathcal{S}$ the derived system $DAE(\mathcal{A}(\tilde{t}_1)/\mathcal{S}_0^*) = DAE(\emptyset)$ fulfills the transversality condition (3.6) starting from $t = \tilde{t}_1$. In other words, inequality constraint (4.4e) is deactivated at $t = \tilde{t}_1$.

At $t = \tilde{t}_2$, the event function $\phi_1(t)$ changes its sign from positive to negative, refer to Fig. 10. This indicates that a continued simulation will violate inequality constraint (4.4d), refer also to Fig. 8. At this time point, $\mathcal{A}(\tilde{t}_2) = \{1\}$, $\mathcal{S} = \{1\}$, and if we choose $\mathcal{S}_0^* = \emptyset$ the derived system $DAE(\mathcal{A}(\tilde{t}_2)/\mathcal{S}_0^*) = DAE(\{1\})$ fulfills the transversality condition (3.6) starting from $t = \tilde{t}_2$. In other words, inequality constraint (4.4d) is activated at $t = \tilde{t}_2$. Simulation continues from $\tilde{t}_2$ until the final simulation time $t_{end} = 2$ is reached.

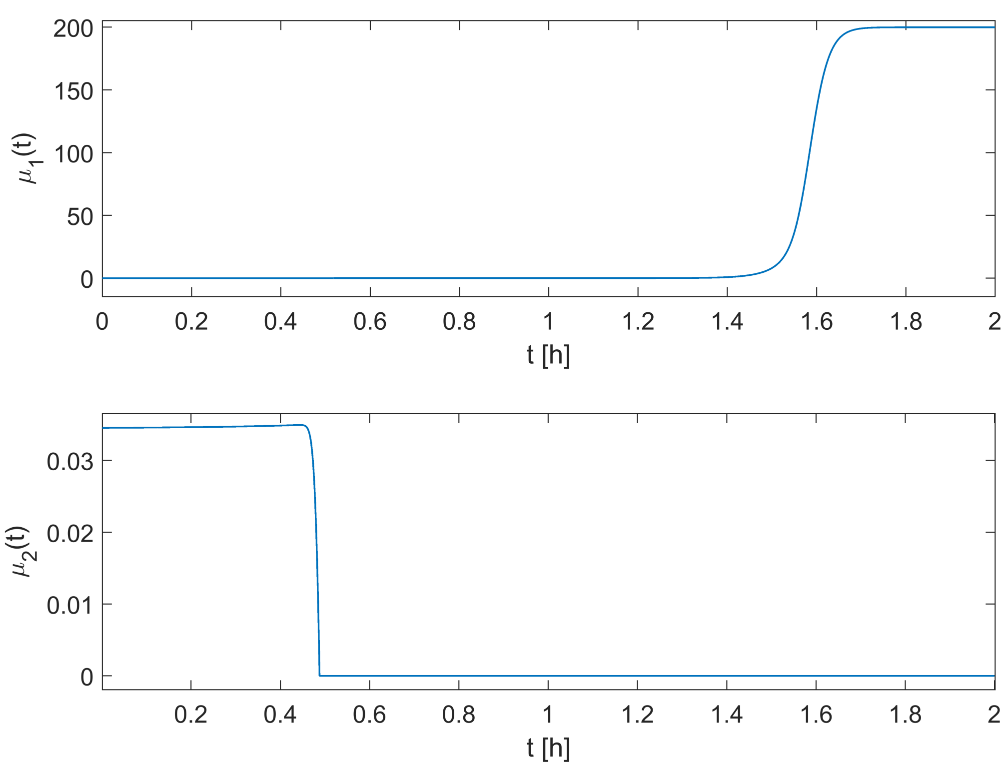

FIGURE 9. Simulation results: Lagrangian multiplier μ_1 and μ_2 for inequality (4.4d) and (4.4e).

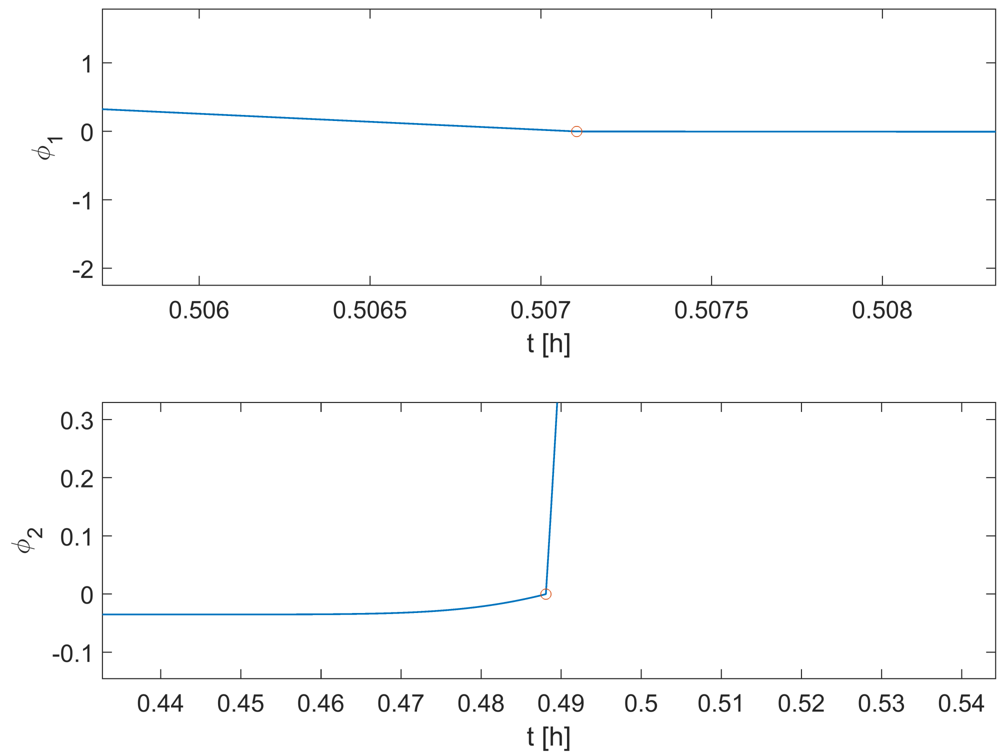

FIGURE 10. Simulation results: Event functions ϕ_1 and ϕ_2 near switching time $\tilde{t}_1$ and $\tilde{t}_2$. Cycles refer to switching times.

4.3. **Implementation.** All simulation results are computed in Matlab environment. Numerical solver *ode*15*s* in Matlab is used to solve the derived DAE systems. Detection of event functions is realized by specifying the "Event Location Property" of the applied DAE solver through command *odeset* in Matlab.

5. CONCLUSION

In this work, we discuss the theoretical solution of OCDE in the form of Eq. (1.2) and propose a numerical algorithm to solve it. The analysis and the solution approach is based on the KKT condition of nonlinear programming, which transforms the original system into a sequence of constructed DAE systems. In order to solve the original OCDE system, one solves this sequence of DAE systems instead.

Sufficient conditions are given at regular KKT points such that in a small neighborhood the solution of the original system is the same as the solution of a derived index-1 DAE system. At non-regular points, where strict complementarity condition is damaged, we construct a new index-1 DAE system such that its solution starts from the non-regular points and corresponds to the solution of the original OCDE. Because the constructed DAE system at non-regular points may have a different formulation, non-smooth points (switching behavior) along the solution trajectory are expected.

To locate the time when switching happens, we propose an event function. Under transversality conditions, it is proved that the proposed event function changes its sign. The proposed solution algorithm has been successfully applied to two examples. One example comes from the case study of simulating bioreactors.

We note that this work is subject to the following limitations. First, the main results of this paper rely on the application of the IFT. In case that, the IFT can not be applied, e.g. violation of Condition (3.3), the derived DAE system may be not index-1 and the proposed solution algorithm may not work. Second, the proposed algorithm is limited to tract only KKT points. There is no guarantee that these KKT points are local minimizers. Third, we consider only deterministic dynamic systems, in the sense that local minimizers of $P(x)$ are locally unique and the solution of OCDE is determined from a given initial condition. If this is not the case, e.g. local minimizers are not unique, one may need the techniques of differential inclusions to analyze the solutions of OCDE. These issues remain open topics for the future.

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APPENDIX

Theorem 1 (Implicit Function Theorem (IFT), refer to e.g. Theorem 2.4.1 in [4])**.** *Suppose* $f : \mathbb{R}^{n+m} \to \mathbb{R}^n$ *is a* k *times continuously differentiable mapping whose domain is* Ω*. Suppose* $(\bar{x}^T, \bar{y}^T)^T \in \Omega$*,* $f(\bar{x}, \bar{y}) = 0$ *and the Jacobian with respect to* x*,* $\nabla_x f(\bar{x}, \bar{y})$*, is non-singular. Then there exists a neighborhood* $U_{\bar{y}}$ *of* $\bar{y}$ *and an unique function* $x : U_{\bar{y}} \to \mathbb{R}^n$*,* $x(\cdot) \in \mathcal{C}^k$*, such that* $x(\bar{y}) = \bar{x}$ *and* $f(x(y), y) = 0$*,* $\forall y \in U_{\bar{y}}$*.*

Lemma 1 (Lemma 2.4.3 in [9])**.** *Let* A *be a symmetric* $n \times n$ *matrix,* B *a* $n \times k$ *matrix and* C *a* $k \times k$ *matrix. Then the matrix*

$$\begin{pmatrix} A & B \\ CB^T & 0 \end{pmatrix}$$

is non-singular, if and only if C *is non-singular, rank* $B = k$ *and* $A|_{KerB^T}$ *is non-singular.*

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