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Continuous-Time Enclosures for Uncertain Implicit Differential Equations

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Abstract: The computation of enclosures for the reachable set of uncertain dynamic systems is a crucial component in a wide variety of applications, from global and robust dynamic optimization to safety verification and fault detection. Even though many systems in engineering are best modeled as implicit differential equations (IDEs) and differential algebraic equations (DAEs), methods for the construction of enclosures for these are not as well developed as they are for ordinary differential equations (ODEs). In this paper, we propose a continuous-time approach for the guaranteed over approximations of the reachable set for quasilinear IDEs. This approach builds on novel high-order inclusion techniques for the solution set of algebraic equations and state-of-the-art techniques for bounding the solution of nonlinear ODEs. We show how this approach can be used to bound the reachable set of uncertain semi-explicit DAEs by bounding the underlying IDEs. We demonstrate this approach on two case studies, a double pendulum where it proves superior with delayed break-down times compared to other methods, and anaerobic digestion of microalgae which has nine differential and two algebraic states.

Keywords: Implicit differential equations; reachable set; differential inequalities; polynomial models; ellipsoidal calculus; high-order inclusions

1. INTRODUCTION

The computation of enclosures of the reachable set of uncertain dynamic systems appear in a great variety of applications, including global and robust dynamic optimization (Chachuat et al., 2006; Houska et al., 2012), robust MPC (Limon et al., 2005), guaranteed state and parameter estimation (Jaulin, 2002; Kieffer and Walter, 2011) and safety verification (Lin and Stadtherr, 2009). Most of the available methods are developed for systems governed by ordinary differential equations (ODEs).

Bounding techniques for parametric/uncertain ODEs can be broadly classified as continuous-time and discrete-time. Discrete-time set propagation methods rely on a two-phase approach (Nedialkov et al., 1999), whereby a domain in which the existence and uniqueness of solutions can be established is computed in the first phase, and a tightened enclosure is then propagated until the end of the current time step in the second phase. Continuous-time methods involve constructing an auxiliary system of ODEs whose solution is guaranteed to enclose the reachable set of the original ODEs. These methods are inspired from the theory of differential inequalities (Walter, 1970), viability theory (Aubin, 1991), or other set-theoretic methods such as ellipsoidal calculus (Houska et al., 2012). Recently, Villanueva et al. (2014) have developed a unifying framework based on a generalized differential inequality for continuous-time propagation of convex and non-convex enclosures of the reachable set of uncertain ODEs.

Often ODEs do not provide the best framework for describing dynamic systems, and implicit differential equations (IDEs) can offer a more natural modeling framework. In contrast to ODEs, some of the state time derivatives in IDEs cannot be explicitly expressed. IDEs often arise in mechanical (Blajer, 1992) and electrical systems (Riaza, 2008). Semi-explicit differential algebraic equations (DAEs) are a special case that combine ODEs with algebraic equations. In chemical engineering, DAEs arise naturally in combining mass and energy balances with thermodynamic relations, or in discretizing time-dependent PDEs with the method of lines (Hangos and Cameron, 2001).

Despite their many applications, methods for reachability analysis for IDEs and DAEs are not as well developed as for ODEs. They can also be classified as either continuous-time or discrete-time, and have been mainly restricted to semi-explicit index-one DAEs. Hoefkens et al. (2003) developed a discrete-time approach for the propagation of Taylor models using differential algebras (Berz and Makino, 1998) through index-one semi-explicit DAEs. Likewise, Rauh et al. (2009) built upon an existing validated discrete-time method for ODEs (Rauh et al., 2006) to address semi-explicit index-1 DAEs through the combination with an interval Krawczyk method for bounding the algebraic constraints. More recently, Scott and Barton (2013) have presented a continuous-time method which combines the theory of differential inequalities with a Newton-type method to handle the algebraic constraints.

In this paper, we present an alternative approach for the continuous-time propagation of reachable set enclosures for uncertain IDEs. This approach combines high-order inclusion techniques for algebraic equations with techniques for bounding the solution of nonlinear ODEs. The paper is organized as follows, a more precise formulation of the problem is given in Sect. 2. High-order inclusion techniques are briefly recalled in Sect. 3, and their extension to address a broad class of IDEs is then presented in Sect. 4. This approach is demonstrated on two case studies in Sect. 5, before concluding the paper in Sect. 6.

2. PROBLEM DEFINITION

We consider implicit differential equations of the form

$$M(x(t,p),p)\,\dot{x}(t,p) = f(x(t,p),p) \tag{1}$$

where $t \in [0,T]$ denotes time; $p \in P \subseteq \mathbb{R}^{n_p}$ the uncertain parameter vector contained in the compact set P; $x : [0,T] \times P \to \mathbb{R}^{n_x}$ the state trajectories; and $M(x(t,p),p) \in \mathbb{R}^{n_x \times n_x}$ is the so-called mass matrix. All functions are assumed to be sufficiently often continuously differentiable. The reachable set of Eq. (1) is defined as

$$X(t) := \{x(t,p) \,|\, p \in P\}. \tag{2}$$

The problem addressed in this paper is that of computing time-varying enclosures $\overline{X}(t) \supseteq X(t)$ using continuous-time set-propagation techniques. Assumptions about M and initial conditions are discussed later in Sect. 4.

2.1 Notation

The set of n-dimensional interval vectors is denoted by $\mathbb{IR}^n$. The midpoint and radius of an interval vector $Z := [z^{\mathrm{L}}, z^{\mathrm{U}}] \in \mathbb{IR}^n$ are defined as $\operatorname{mid} Z := \frac{1}{2}(z^{\mathrm{U}} + z^{\mathrm{L}})$ and $\operatorname{rad} Z := \frac{1}{2}(z^{\mathrm{U}} - z^{\mathrm{L}})$, respectively. The set of n-dimensional positive-semidefinite matrices is denoted by $\mathbb{S}^n_+$. An ellipsoid with shape matrix $Q \in \mathbb{S}^n_+$ and centered at the origin is denoted by $\mathcal{E}(Q) := \{Q^{\frac{1}{2}} v \,|\, v \in \mathbb{R}^n, v^{\mathsf{T}} v \leq 1\}$. A q-th order polynomial model of a function $h : \mathbb{R}^n \to \mathbb{R}^m$ on a compact subset $Z \subseteq \mathbb{R}^n$ is defined as the pair $\mathcal{M}^q_h := (\mathcal{P}^q_h, \mathcal{R}^q_h)$, with $\mathcal{P}^q_h : \mathbb{R}^n \to \mathbb{R}^m$ a q-th order multivariate polynomial and a convex compact set $\mathcal{R}^q_h \subseteq \mathbb{R}^m$ satisfying $h(z) - \mathcal{P}^q_h(z) \in \mathcal{R}^q_h$ for $z \in Z$. One class of polynomial models is that of Taylor models, whereby the polynomial coincides with the Taylor expansion of the function up to order q (Neumaier, 2003). Other classes of polynomial model can be constructed using orthogonal polynomial such as expansion in Chebyshev basis.

3. CONTINUOUS-TIME SET PROPAGATION FOR ORDINARY DIFFERENTIAL EQUATIONS

As a special case of Eq. (1), when $M(x(t,p),p)$ is the identity matrix, the problem reduces to bounding a system of ODEs. We provide a brief overview of some existing continuous-time propagation methods for uncertain ODEs. We focus on methods with high-order convergence in the Hausdorff sense via propagation of polynomial models with interval or ellipsoidal remainders (Villanueva et al., 2014). A point-wise in time polynomial model enclosure of the reachable set is defined as

$$\overline{X}(t) := \{\mathcal{P}^q_x(t,p) \,|\, p \in P\} \oplus \mathcal{R}^q_x(t). \tag{3}$$

The polynomial part $\mathcal{P}^q_x$ is constructed by propagating the monomial coefficients through ODEs via the application of arithmetic rules for polynomial models. In the case of Taylor models, for instance, these ODEs correspond to the sensitivity equations up to order q. An interval remainder $\mathcal{R}^q_x(t) := \left[r^{\mathrm{L}}_x(t), r^{\mathrm{U}}_x(t)\right]$ can be propagated by integrating the following $2 \times n_x$ system of auxiliary ODEs:

$$\dot{r}^{\mathrm{L}}_i(t) = \min_{\xi,\rho} \left\{ \begin{array}{l|l} f_i(\mathcal{P}^q_x(t,\rho)+\xi,\rho) & \xi_i = r^{\mathrm{L}}_{x_i}(t) \\ \quad - \dot{\mathcal{P}}^q_{x_i}(t,\rho) & \xi \in [r^{\mathrm{L}}_x(t), r^{\mathrm{U}}_x(t)] \\ & \rho \in P \end{array} \right\} \tag{4}$$

$$\dot{r}^{\mathrm{U}}_i(t) = \max_{\xi,\rho} \left\{ \begin{array}{l|l} f_i(\mathcal{P}^q_x(t,\rho)+\xi,\rho) & \xi_i = r^{\mathrm{U}}_{x_i}(t) \\ \quad - \dot{\mathcal{P}}^q_{x_i}(t,\rho) & \xi \in [r^{\mathrm{L}}_x(t), r^{\mathrm{U}}_x(t)] \\ & \rho \in P \end{array} \right\} \tag{5}$$

for all $i \in \{1, \ldots, n_x\}$.

An ellipsoidal enclosure $\mathcal{E}(Q^q_x(t))$ of the qth-order remainder term can be created by integrating an $n_x \times n_x$ system of auxiliary ODEs:

$$\begin{aligned} \dot{Q}^q_x(t) = A(t)Q^q_x(t) + Q^q_x(t)A(t)^{\mathsf{T}} + \sum_{i=1}^{n_x} \kappa_i(t)\, Q^q_x(t) \\ + \operatorname{diag}(\kappa(t))^{-1} \operatorname{diag}\operatorname{rad}(\Omega^q_f[Q^q_x(t)])^2\,, \end{aligned} \tag{6}$$

with $A(t) := \left(\frac{\partial f}{\partial x}(\mathcal{P}^q_x(t,\hat{p}),\hat{p})\right)$. At a given time t, the nonlinearity bounder $\Omega^q_f[Q] \in \mathbb{IR}^{n_x}$ must satisfy

$$f(\mathcal{P}^q_x(t,\rho)+r,\rho) - \dot{\mathcal{P}}^q_x(t,\rho) - \frac{\partial f}{\partial x}(\mathcal{P}^q_x(t,\rho),\rho)\, r \in \Omega^q_f[Q],$$

for all $(r,\rho) \in \mathcal{E}(Q) \times P$, and it can be automatically constructed using interval analysis. The scaling function $\kappa : [0,T] \to \mathbb{R}^{n_x}_{++}$ can be chosen to minimize $\operatorname{tr}(Q^q_x(t))$. Overall, computing reachable set enclosures as $\{\mathcal{P}^q_x(t,p) \mid p \in P\} \oplus \left[r^{\mathrm{L}}_x(t), r^{\mathrm{U}}_x(t)\right]$ and $\{\mathcal{P}^q_x(t,p) \mid p \in P\} \oplus \mathcal{E}(Q^q_x(t))$ calls for the solution of auxiliary bounding systems with, respectively, $O(n_x n^q_p)$ and $O(n_x n^q_p + n^2_x)$ ODEs.

4. CONTINUOUS-TIME SET-PROPAGATION FOR IMPLICIT DIFFERENTIAL EQUATIONS

We now consider Eq. (1) with a general mass matrix M. We will apply the *same* high-order set-propagation techniques as in Sect. 3. When M is structurally non-singular, there are two approaches:

i) via symbolic manipulation, by reformulating Eq. (1) into a system of ODEs. Expressions for $M(x,p)^{-1}f(x,p)$ can be obtained by applying Gaussian elimination symbolically, involving a finite number of steps.
ii) via numerical evaluation, by computing high-order inclusions, for given sets P and X, of the form

$$\Xi := \{\xi \,|\, M(x,p)\xi = f(x,p), p \in P, x \in X\}. \tag{7}$$

Then use then to evaluate the right-hand sides of the auxiliary bounding systems in Eqs. (4)-(5) or (6).

The former approach is straightforward but may yield poor enclosures on $X(t)$ when no preconditioning is used in the symbolic inversion of M. The effect of preconditioning is known to be critical for computing tight bounds on the solutions of implicit equations (Neumaier, 1990). The focus in this work is therefore on the second approach, and

techniques for computing high-order inclusions of sets such as in Eq. (7) will be presented later in Sect. 4.1.

When the matrix M is structurally singular, Eq. (1) represents a system of DAEs that can be rewritten in linear implicit form:

$$M_D(x(t,p),p)\,\dot{x}(t,p) = f_D(x(t,p),p) \tag{8a}$$
$$0 = f_A(x(t,p),p)\,, \tag{8b}$$

with

$$M =: \begin{pmatrix} M_D \\ 0 \end{pmatrix}, \quad \text{and} \quad f =: \begin{pmatrix} f_D \\ f_A \end{pmatrix}.$$

Inverting M, symbolically or numerically, would fail but we can derive the underlying (implicit) ODEs by differentiating the algebraic part (8b) with respect to time, giving

$$\frac{\partial f_A}{\partial x}(x(t,p),p)\,\dot{x}(t,p) = 0. \tag{9}$$

A sufficient condition for the DAE system (8) to have index one is when the matrix $M^{(1)}$ defined below remains non-singular along the time horizon $[0,T]$ (Riaza, 2008):

$$M^{(1)} := \begin{pmatrix} M_D \\ \dfrac{\partial f_A}{\partial x} \end{pmatrix}.$$

If $M^{(1)}$ is structurally singular, meaning that the DAE system is high index, we can repeat the differentiation process on part of Eq. (9), similar to classical index-reduction techniques (Mattsson and Soderlind, 1993). After this transformation, high-order inclusions of the solutions of the underlying (implicit) ODEs are computed as shown earlier for

$$M^{(k)}(t,x(t,p),p)\,\dot{x}(t,p) = \begin{pmatrix} f_D(x(t,p),p) \\ 0 \end{pmatrix}, \tag{10}$$

with k the differentiation index.

4.1 High-Order Inclusions of State Time Derivatives

The implicit ODEs (1) (or underlying ODEs (10)) are linear in state time derivatives and can be rewritten as

$$A(y)\xi = b(y)\,, \tag{11}$$

where $y \in \mathbb{R}^{n_y}$ is the vector of independent variables corresponding to the states and parameters (x,p) in Eq. (1), and $\xi \in \mathbb{R}^{n_x}$, a vector of the dependent variables corresponding to the state time derivatives $\dot{x}$. We assume that $A : \mathbb{R}^{n_y} \to \mathbb{R}^{n_x \times n_x}$ and $b : \mathbb{R}^{n_y} \to \mathbb{R}^{n_x}$ are sufficiently often continuously differentiable in their arguments such that A and b can be evaluated in polynomial model arithmetic. A also has to be non-singular for every value of y.

Methods for computing interval bounds on the solutions of implicit equations are well developed (see, e.g., Neumaier, 1990). Here we focus on high-order inclusions of the implicit solutions, to combine with the high-order continuous-time methods discussed in Sect. 3. We wish to create a polynomial model $\mathcal{M}_\xi(p)$ for the dependent variables ξ on P, given a polynomial model $\mathcal{M}_y(p)$ of the independent variables. One way, which does not require an initial guess for the solution set, is an extension of Gaussian elimination with operations carried out using polynomial model arithmetic. The first step involves preconditioning the system (11) as

$$\mathcal{M}^q_{\mathsf{G}}(p)\,\xi = \mathcal{M}^q_c(p)\,, \tag{12}$$

with $\mathcal{M}^q_{\mathsf{G}}(p) := \mathsf{Y}\cdot\mathcal{M}^q_A(p)$ and $\mathcal{M}^q_c(p) := \mathsf{Y}\cdot\mathcal{M}^q_b(p)$, where $\mathsf{Y} \in \mathbb{R}^{n_x\times n_x}$ is any preconditioning matrix, often the inverse of the mid-point of an interval enclosure of $\mathcal{M}^q_A(y)$, and $\mathcal{M}^q_b(p)$ and $\mathcal{M}^q_A(p)$ are the polynomial model extensions of $b(y)$ and $A(y)$, respectively. In the second step, the matrix $\mathcal{M}^q_{\mathsf{G}}(p)$ is converted to upper-triangular form and back-solved from the bottom row up for $\mathcal{M}^q_\xi(p)$.

Bounds can be refined using an iterative method such as Gauss-Seidel, however Gaussian elimination alone can be sufficient for problems with a small number of independent variables. For a polynomial model $\mathcal{M}^k_\xi(p) := (\mathcal{P}^k_\xi(p), \mathcal{R}^k_\xi)$—we use the superscript k here to refer to the iteration number—a new model $\mathcal{M}^{k+1}_\xi(p)$ can be constructed with the following iteration—see, Rajyaguru and Chachuat (2013), for more details:

$$\forall i \in \{1,\ldots,n_x\}: \tag{13}$$
$$\mathcal{M}^{k+1}_{\Gamma_i}(p) := \mathcal{P}^k_{\xi_i}(p) - \frac{1}{\mathcal{M}^q_{\mathsf{G}_{i,i}}(p)}\Bigg[\mathcal{M}^q_{c_i}(p) + \sum_{j=1}^{i-1}\left[\mathcal{M}^q_{\mathsf{G}_{i,j}}\cdot(\mathcal{M}^{k+1}_{\xi_j} - \mathcal{P}^k_{\xi_j})\right](p) + \sum_{j=i+1}^{n_x}\mathcal{M}^q_{\mathsf{G}_{i,j}}(p)\cdot\mathcal{R}^k_{\xi_j}\Bigg]$$
$$\mathcal{M}^{k+1}_{\xi_i}(p) := \left(\mathcal{P}^{k+1}_{\Gamma_i}(p),\ \mathcal{R}^{k+1}_{\Gamma_i} \cap [\mathcal{P}^k_{\xi_i} - \mathcal{P}^{k+1}_{\Gamma_i}](P) + \mathcal{R}^k_{\xi_i}\right).$$

We use the polynomial model for ξ provided by Gaussian elimination as the initial iterate $\mathcal{M}^0_\xi(p)$.

4.2 High-Order Inclusions of Initial Conditions

When M in Eq. (1) is structurally singular, consistent initial conditions must be computed for the algebraic part (8b). In the case of index-1 DAEs, and assuming that initial conditions are provided for a subset of the states x_D, computing a polynomial model of the remaining states x_A involves solving an implicit nonlinear algebraic system,

$$g(\zeta,\eta) = 0\,, \tag{14}$$

with $\zeta := x_A$, $\eta := [x_D^{\mathrm{T}}\ p^{\mathrm{T}}]^{\mathrm{T}}$ and $g := f_A$.

The Gauss-Seidel iteration (13) for implicit equations linear in the dependent variables can be extended to compute such a polynomial model. Notice that $A(y)$ and $b(y)$ are replaced with $\frac{\partial g}{\partial\zeta}(\zeta,\eta)$ and $g(\zeta,\eta)$, respectively. Due to the nonlinearity, it is beneficial to update the preconditioning matrix at each iteration now,

$$\mathcal{M}^q_{\frac{\partial g}{\partial\zeta}}(\mathcal{P}^k_\zeta(p) + [0,1]\cdot\mathcal{R}^k_\zeta(p), \mathcal{P}^q_\eta(p))\,,$$

so both $\mathcal{M}^q_c(p)$ and $\mathcal{M}^q_{\mathsf{G}}(p)$ are now replaced with the iteration dependent $\mathcal{M}^k_c(p)$ and $\mathcal{M}^k_{\mathsf{G}}(p)$ as

$$\mathcal{M}^k_c(p) := \mathsf{Y}^k\cdot\mathcal{M}^q_g(\mathcal{P}^k_\zeta(p), \mathcal{P}^q_\eta(p))$$
$$\mathcal{M}^k_{\mathsf{G}}(p) := \mathsf{Y}^k\cdot\mathcal{M}^q_{\frac{\partial g}{\partial\zeta}}(\mathcal{P}^k_\zeta(p) + [0,1]\cdot\mathcal{R}^k_\zeta, \mathcal{P}^q_\eta(p))\,.$$

A complication with nonlinear algebraic systems is that it is no longer possible to use Gaussian elimination to get an initial valid enclosure $\mathcal{M}^0_\zeta(p)$. Therefore, some conservative initial bounds must be provided for the algebraic variables.

5. NUMERICAL CASE STUDIES

The method developed in the previous section is applied to two problems, a mechanical double-pendulum that is described by IDEs (4 states), and an anaerobic

digester for processing microalgal biomass that is described by index-1, semi-explicit DAEs (11 states, 2 algebraic constraints). We have implemented the method in a C++ program, using our in-house implicit equation solver (AEBND) and continuous-time integrator (ODEBND, Villanueva et al., 2014). The latter relies on the explicit ODE solvers with adaptive step-size control available as part of the GNU Scientific Library (GSL), linked to the library MC++ (`https://projects.coin-or.org/MCpp`) implementing both Taylor and Chebyshev model arithmetics. In the both case studies we use the explicit embedded Runge-Kutta-Fehlberg (4,5) method in GSL, with relative tolerance of 10^{-7} and absolute tolerance of 10^{-8}. The implicit equation solver uses Gaussian elimination to initialize a Gauss-Seidel iteration, here with a maximum of 20 iterations and a relative stopping tolerance of 10^{-7}. CPU times are not reported for the case studies since the implementation is not yet optimized and presents much room for improvement. Break-down times reported in this section refer to when the step-size would be smaller than 10^{-6} of corresponding time units, an indication of when numerical integration approaches an escape time.

5.1 Double Pendulum

Modeling of constrained mechanical systems using Lagrangian mechanics often gives rise to IDEs. We consider a planar pair of connected pendula in a frictionless environment. Assuming that both pendula are massless and rigid, with point masses on the ends, this problem reduces to the following 4-dimensional ODE:

$$\begin{aligned}
0 &= \dot{\psi}_1 - \psi_3 \\
0 &= \dot{\psi}_2 - \psi_4 \\
0 &= [m_1 l_1 + m_2(l_1 + l_2\cos(\psi_2))]\dot{\psi}_3 + m_2 l_2 \cos(\psi_2)\dot{\psi}_4 \\
&\quad + g(m_1+m_2)\sin(\psi_1) - m_2 l_2 \sin(\psi_2)[\psi_3+\psi_4]^2 \\
0 &= m_2(l_1\cos(\psi_2) + l_2)\dot{\psi}_3 + m_2 l_2 \dot{\psi}_4 + g\, m_2 \sin(\psi_1+\psi_2) \\
&\quad + m_2 l_1 \sin(\psi_2)(\psi_3)^2 \,,
\end{aligned}$$

in the angles ψ_1, ψ_2 and angular velocities ψ_3, ψ_4. In this instance, we consider uncertain initial conditions

$$\psi_1(0) = \frac{3\pi}{4}p\,, \quad \psi_2(0) = -\frac{11\pi}{20}\,, \quad \psi_3(0) = 0.43\,,$$
$$\text{and} \quad \psi_4(0) = 0.67\,,$$

with $p \in [0.99, 1.01]$. Enclosures of the state variables obtained by applying the approach in Sect. 4 are shown in Fig. 1 (in projection), here by propagating Chebyshev models of orders 1, 3, 5 and 7 with ellipsoidal remainders — interval remainders lead to weaker bounds. The bounds are seen to approximate the actual solution set (grey area) very closely. The break-down times of the algorithm are progressively delayed as the expansion order is increased. For expansion order of 7 or higher the improvement becomes marginal.

In carrying out a comparative study for this example by reformulating the system as explicit ODEs, Rauh et al. (2006) found that the usual methods based on interval arithmetic break down before $t \leq 1$. Likewise, the validated integrator Cosy Infinity (version 9) by Makino and Berz (2006), which propagates Taylor models, breaks down around $t = 2$ even for 12th-order Taylor expansions. The proposed approach is thus superior on this example.

5.2 Anaerobic Digestion of Microalgae

The modeling of bioprocesses often gives rise to challenging dynamic systems, whereby differential equations describing species mass balances in the system are coupled with algebraic equations describing charge balance or other fast phenomena that are assumed to be at equilibrium (quasi steady-state). We consider a three-reaction model of anaerobic digestion of microalgae inspired from (Mairet et al., 2012). This model involves two hydrolysis+acetogenesis steps in parallel, whereby sugars+lipids (S_1) and protein (S_2) are converted into VFA (S_3), followed by a methanogenic step; each reaction is associated with a specific bacterial population X_1, X_2 or X_3:

- hydrolysis+acetogenesis of sugars+lipids:
$$\alpha_1\, S_1 + \alpha_2\, \mathrm{NH_4^+} \overset{\mu_1(\cdot)\, X_1}{\longrightarrow} X_1 + \alpha_3\, S_3 + \alpha_4\, \mathrm{CO_2}$$
- hydrolysis+acetogenesis of proteins:
$$\alpha_5\, S_2 \overset{\mu_2(\cdot)\, X_2}{\longrightarrow} X_2 + \alpha_6\, S_3 + \alpha_7\, \mathrm{NH_4^+} + \alpha_8\, \mathrm{CO_2}$$
- methanogenesis:
$$\alpha_9\, S_3 + \alpha_{10}\, \mathrm{NH_4^+} \overset{\mu_3(\cdot)\, X_3}{\longrightarrow} X_3 + \alpha_{11}\, \mathrm{CH_4} + \alpha_{12}\, \mathrm{CO_2}$$

The biological kinetics for these reactions are

$$\mu_1(S_1) = \bar{\mu}_1 \frac{S_1}{S_1 + K_{S1}}, \quad \mu_2(S_2) = \bar{\mu}_2 \frac{S_2}{S_2 + K_{S2}},$$
$$\mu_3(S_3, \mathrm{NH_3}) = \bar{\mu}_3 \frac{S_3}{S_3 + K_{S3} + \frac{S_3^2}{K_{I3}}} \frac{K_{I_{\mathrm{NH_3}}}}{K_{I_{\mathrm{NH_3}}} + \frac{K_N}{h + K_N} N}.$$

Under perfect mixing, the species-balance equations for the state variables S_1, X_1, S_2, X_2, S_3, X_3, inorganic nitrogen (N), inorganic carbon (C), and alkalinity (Z):

$$\begin{aligned}
\dot{S}_1 &= D(\beta_1 S^{\mathrm{in}} - S_1) - \alpha_1 \mu_1 X_1 \\
\dot{X}_1 &= (\mu_1 - D) X_1 \\
\dot{S}_2 &= D(\beta_2 S^{\mathrm{in}} - S_2) - \alpha_5 \mu_2 X_2 \\
\dot{X}_2 &= (\mu_2 - D) X_2 \\
\dot{S}_3 &= -D\, S_3 + \alpha_3 \mu_1 X_1 + \alpha_6 \mu_2 X_2 - \alpha_9 \mu_3 X_3 \\
\dot{X}_3 &= (\mu_3 - D) X_3 \\
\dot{N} &= D(N^{\mathrm{in}} - N) - \alpha_2 \mu_1 X_1 + \alpha_7 \mu_2 X_2 - \alpha_{10} \mu_3 X_3 \\
\dot{C} &= D(C^{\mathrm{in}} - C) + \alpha_4 \mu_1 X_1 + \alpha_8 \mu_2 X_2 + \alpha_{12} \mu_3 X_3 - q_{\mathrm{CO_2}} \\
\dot{Z} &= D(Z^{\mathrm{in}} - Z)
\end{aligned}$$

with D, the dilution rate; and S^{in}, N^{in}, C^{in} and Z^{in}, the inlet concentrations. Note that these balances neglect gaseous emissions of ammonia and VFAs. The following charge-balance equation assumes that all acid/base pairs are in equilibrium with $h := 10^{-\mathrm{pH}}$, and that the pH range of operation is lower than 8:

$$\begin{aligned}
Z + h + \frac{h}{h + K_N} N - \frac{K_C}{K_C + h} C \\
- \frac{K_{\mathrm{VFA}}}{\gamma_{\mathrm{VFA}}(K_{\mathrm{VFA}} + h)} S_3 - \frac{K_{\mathrm{H_2O}}}{h} = 0\,,
\end{aligned}$$

with K_C, K_N, K_{VFA} and $K_{\mathrm{H_2O}}$, the dissociation constants for $\mathrm{HCO_3^-/CO_2}$, $\mathrm{NH_3/NH_4^+}$, $\mathrm{VFA^-/HVFA}$ and water, respectively; and $\gamma_{\mathrm{VFA}} = 64\,\mathrm{g_{COD}\,mol^{-1}}$, by assimilating VFA to pure acetate. Finally, assuming that the partial pressures of $\mathrm{CO_2}$ ($P_{\mathrm{CO_2}}$) and methane ($P_{\mathrm{CH_4}}$) quickly reach equilibrium and the gas behaves ideally, we have:

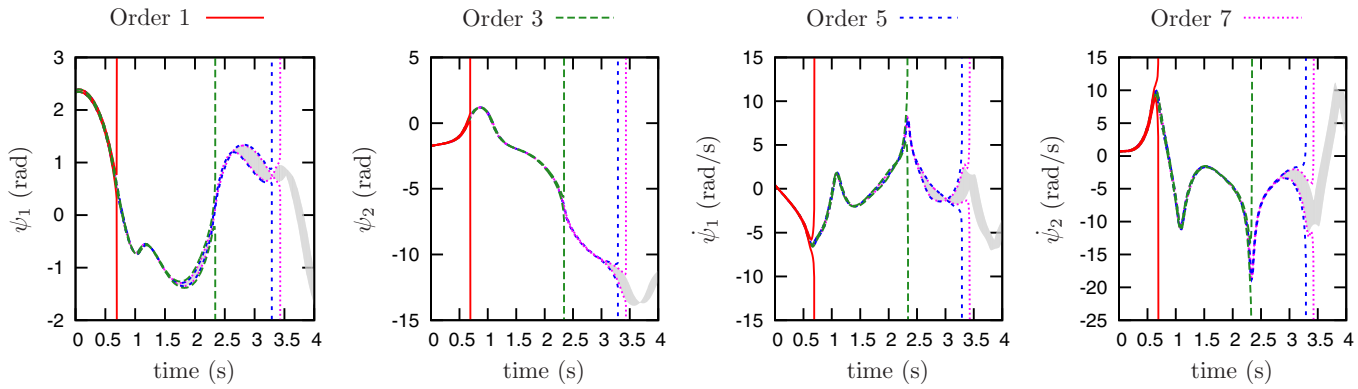

Fig. 1. Computed trajectory bounds for double-pendulum problem.

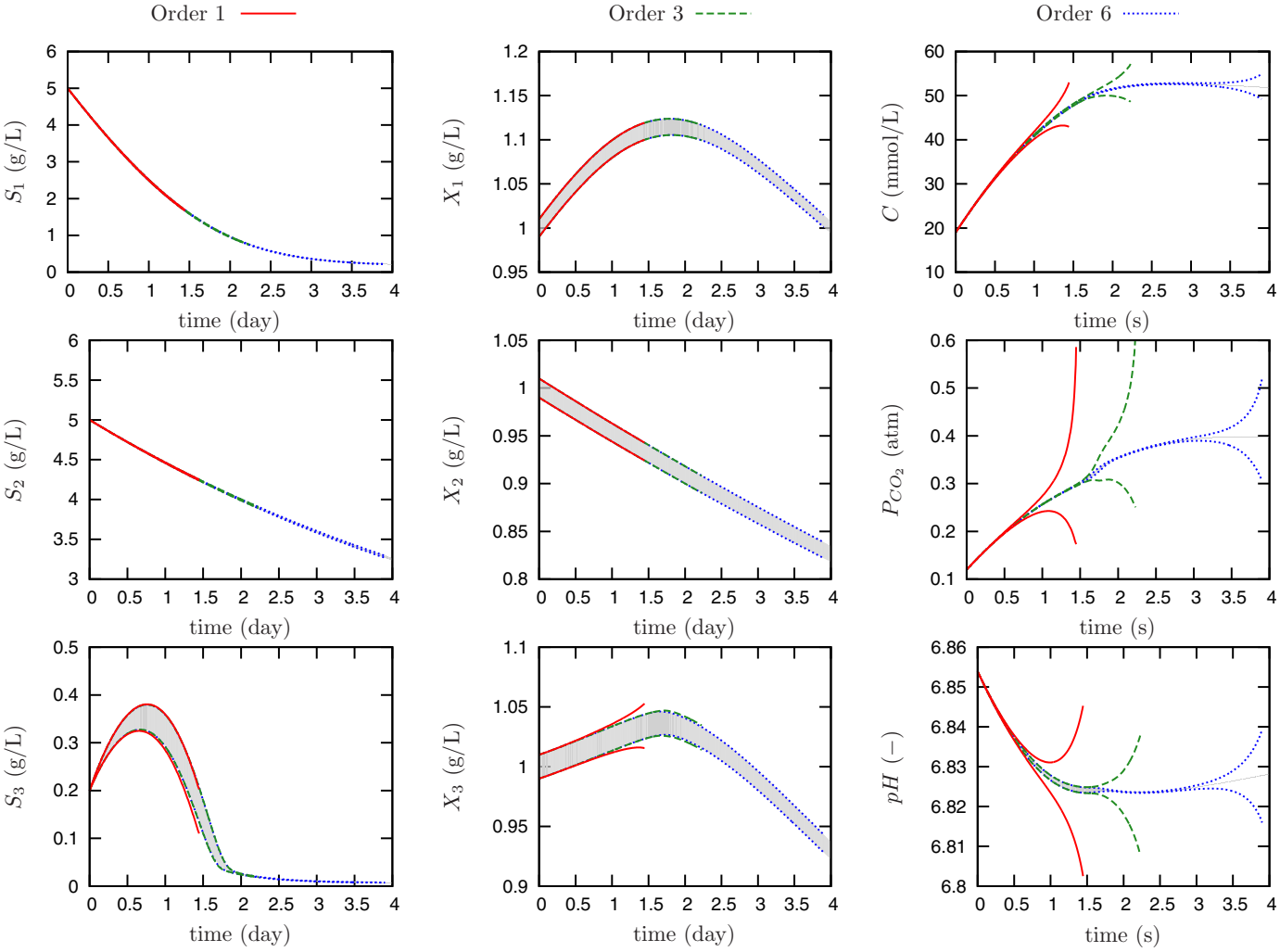

Fig. 2. Computed trajectory bounds for anaerobic digestion of microalgae.

$$\frac{P_{\text{tot}} - P_{\text{CO}_2}}{q_{\text{CH}_4}} = \frac{P_{\text{CO}_2}}{q_{\text{CO}_2}},$$

where the liquid-gas transfer rates are given by:

$$\begin{aligned} q_{\text{CH}_4} &= \alpha_{11}\mu_3 X_3 \\ q_{\text{CO}_2} &= k_l a \left(\frac{h}{K_C + h} C - K_{\text{H,CO}_2} P_{\text{CO}_2} \right), \end{aligned}$$

with $K_{\text{H,CO}_2}$, Henry's constant for CO_2, and $k_l a$, the liquid-gas transfer coefficient. The overall anaerobic digestion model is comprised of 9 differential equations/states $(S_1, S_2, S_3, X_1, X_2, X_3, N, C, Z)$ and 2 algebraic equations/states (h, P_{CO_2}). The values of the parameters are as in Mairet et al. (2012, Table II), and the dilution rate, influent concentrations, and total pressure are taken as

$$D = 0.1\ \text{day}^{-1}, \quad S^{\text{in}} = 10\ \text{g L}^{-1}, \quad N^{\text{in}} = 11\ \text{mmol L}^{-1}$$
$$C^{\text{in}} = 19\ \text{mmol L}^{-1}, \quad Z^{\text{in}} = 17\ \text{mmol L}^{-1}, \quad P_{\text{tot}} = 1\ \text{bar}.$$

In this instance, we consider uncertain initial conditions of ±1% for the three initial biomass concentrations as

$X_1(0), X_2(0), X_3(0) \in [0.99, 1.01]$ g L^{-1}; that is, the problem has 3 uncertain parameters. The other initial conditions are $S_1(0) = S_2(0) = 5$ g L^{-1}, $S_3(0) = 0.2$ g L^{-1}, $N(0) = N^{\text{in}} = 11$ mmol L^{-1}, $C(0) = C^{\text{in}} = 19$ mmol L^{-1}, and $Z(0) = Z^{\text{in}} = 17$ mmol L^{-1}, whereas consistent initial conditions for h and P_{CO_2} are computed per the discussion in Sect. 4.2.

Enclosures of the state variables, as obtained by applying the approach in Sect. 4 are shown in Fig. 2 (in projection), here by propagating Chebyshev models of orders 1, 3, and 6 with interval remainders. The computed bounds are seen to approximate the actual solution set (grey area) tightly, and the break-down times of the bounding systems are again progressively delayed as the Chebyshev expansion order is increased.

6. CONCLUSION

In this paper we have presented a new approach for the continuous-time propagation of reachable set enclosures for uncertain implicit differential equations. We have demonstrated this approach on two case studies where for one we have managed to delay the break-down time compared to other approaches and we have managed to obtain the reachable tube for a challenging system with nine differential and two algebraic states. The approach itself is similar to one presented in Hoefkens et al. (2003), where they also differentiate and solve underlying IDEs, however the approach presented here relies on continuous-time set propogation rather than a discrete fixed-point iteration approach.

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