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Interval methods as a simulation tool for the dynamics of biological wastewater treatment processes with parameter uncertainties ☆

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A B S T R A C T

This paper presents sophisticated interval algorithms for the simulation of discrete-time dynamical systems with bounded uncertainties of both initial conditions and system parameters. Since naive implementations of interval algorithms might lead to guaranteed enclosures of all system states which are too conservative to be practically useful, we present algorithmic extensions of classical approaches which are applicable to the simulation of non-cooperative systems with time-varying uncertain parameters. Overestimation arising in the interval evaluation of dynamical system models due to the wrapping effect is reduced by an exact pseudo-linear transformation of nonlinear state equations and by new heuristics for the subdivision of interval enclosures which especially prefer splitting of unstable intervals. To highlight the typical procedure for parameterization of interval-based simulation routines and to demonstrate their efficiency, a nonlinear model of biological wastewater treatment processes is discussed. For this application, we consider the maximum specific growth rate of substrate consuming bacteria as a time-varying uncertain parameter. Only worst-case bounds are assumed to be available for the range of this parameter while no information is provided about its actual variation rate.

1. Introduction

Verified numerics based on interval arithmetic methods provide efficient computational techniques for the simulation of nonlinear dynamical systems with time-varying uncertain parameters. In this contribution, an outline of interval arithmetic simulation algorithms is given. New procedures for the evaluation of discrete-time system models are developed to reduce overestimation in the state enclosures by an exact pseudo-linear transformation of nonlinear state equations accompanied by a routine for the subdivision of interval enclosures which exploits local stability properties of the mathematical system model. This subdivision strategy improves the efficiency of classical verified approaches which are applicable to the evaluation of both static and dynamic systems [1]. To highlight the advantages of these new features, simulation results are presented for a simplified uncertain model of biological wastewater treatment processes.

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Such processes are characterized by uncertainties of several system parameters. These uncertainties are caused by variations of composition and amount of influent wastewater as well as effects of various temperature and weather conditions leading to significant changes of decay and growth rates of the bacteria responsible for water purification. In contrast to traditional simulation techniques like gridding and Monte-Carlo simulations [2], the presented interval arithmetic approach is capable of providing guaranteed bounds of the range of all state variables by taking into account time-varying uncertain system parameters as well as uncertain initial conditions [3]. Since direct measurements of most of the parameters of wastewater treatment processes are either very unreliable or not possible at all, model-based state estimation techniques are essential for the implementation of suitable robust control strategies taking into account parameter uncertainties. Additionally, reliability as well as safety of the plant operation can be analyzed using interval techniques by computation of guaranteed worst-case bounds of all system states. Based on this information, the wastewater treatment process can be optimized with respect to the cost-effectiveness of plant operation.

In contrast to the applications which are, for example, studied in [4,5], our system model does not allow for direct exploitation of cooperativity, that is monotonicity of the solution of the state equations with respect to uncertain parameters or uncertain initial conditions. The main reasons are the structure of the state equations and uncertainties as well as the fact that only worst-case bounds for the range of the uncertain parameter are assumed to be known while no a-priori information about its variation with respect to time is available. Therefore, arbitrary parameter variations between two subsequent time steps have to be taken into account in a verified simulation of the discrete-time dynamical system model.

In general, it is possible to distinguish between the simulation of discrete-time systems which are described by sets of difference equations, usually given in state-space representation, and continuous-time systems described by sets of ordinary differential equations. The focus of this paper is the analysis of discrete-time systems. For that purpose, the considered continuous-time model of a simplified biological wastewater treatment process is replaced by a discrete-time formulation, where the resulting discretization error is neglected.

The choice for simulation of a discretized system model is motivated by the fact that this description is commonly used to design discrete-time control laws for continuous-time real-world processes. Therefore, the analysis of the influence of parameter uncertainties and parameter variations on the state variables of discrete-time systems is the prerequisite for the design of reliable and sufficiently robust controllers. Further simulation routines which are based on verified initial value problem solvers for sets of ordinary differential equations such as VNODE [6–8], COSY VI [9], or ValEncIA-IVP [10] have been studied in detail by the authors in [11] to quantify also the influence of discretization errors in a guaranteed way.

Applying interval techniques may lead to non-negligible overestimation caused by the well-known wrapping effect which arises if non-axis-parallel regions in the state-space are replaced by axis-parallel enclosures in each simulation step of the evaluation of a dynamical system model [1,7]. Sophisticated splitting and merging strategies are implemented to reduce overestimation with suitable computational effort. Efficiency of splitting is further improved by distinguishing between intervals in which the nonlinear system model is locally stable or unstable. Since overestimation often increases faster for unstable than for stable state intervals, they are preferred for splitting. The required stability analysis can be simplified for systems with a known upper bound on the number of unstable eigenvalues. This approach is demonstrated for the subsystem model of biological wastewater treatment which is considered in this paper. Using an interval evaluation of the Routh criterion [12] after linearization of the state equations for all possible operating conditions, it can be proven numerically that this system has at most one unstable eigenvalue. This information significantly reduces the effort that is necessary for the evaluation of the stability-based subdivision criteria.

In Sections 2 and 3, we summarize the main definitions, rules, and properties of interval computation. In Section 4, the applied interval simulation algorithms including new features for the reduction of overestimation based on splitting and merging of interval boxes are described. Section 5 introduces extensions of interval simulation techniques like splitting of unstable intervals. Furthermore, possibilities for the simplification of the stability analysis of systems with a known upper bound on the number of unstable eigenvalues are presented in detail. Several practically relevant settings of the interval arithmetic simulation algorithm are compared to highlight the typical procedure for parameterization of the interval routines under consideration for a subsystem model of biological wastewater treatment processes in Section 6. A prototypical implementation of the proposed simulation techniques as a prognosis software in an industrial process control system is presented in Section 7. Finally, conclusions and an outlook on future research are given in Section 8.

2. Simulation of dynamical systems

In this article, interval methods for simulation of uncertain nonlinear dynamical systems are considered.

For simulation purposes, continuous-time systems

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

with the state vector $x \in \mathbb{R}^{n_x}$ and the uncertain parameter vector $p \in \mathbb{R}^{n_p}$ are replaced by discrete-time models which are, for example, calculated by the explicit Euler method

$$x_{k+1} = x_k + \Delta t \cdot g(x_k, p_k, kT) = f(x_k, p_k, k), \tag{2}$$

with a fixed integration step-size Δt, that is, $t = k\Delta t$. Here effects of unavoidable time discretization errors are neglected. This type of discretization is common practice for the design of discrete-time control strategies for continuous-time systems.