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Qualitative simulation and related approaches for the analysis of dynamic systems

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Abstract

Methods for qualitative simulation allow predictions on the dynamics of a system to be made in the absence of quantitative information, by inferring the range of possible qualitative behaviors compatible with the structure of the system. This article reviews QSIM and other qualitative simulation methods. It discusses two problems that have seriously compromised the application of these methods to realistic problems in science and engineering: the occurrence of spurious behavior predictions and the combinatorial explosion of the number of behavior predictions. In response to these problems, related approaches for the qualitative analysis of dynamic systems have emerged: qualitative phase-space analysis and semi-quantitative simulation. The article argues for a synthesis of these approaches in order to obtain a computational framework for the qualitative analysis of dynamic systems. This should provide a solid basis for further upscaling and for the development of model-based reasoning applications of a wider scope.

1 Introduction

Mathematical modeling is a basic ingredient of research in practically every domain of science and engineering. A quick scan of the July 2002 issue of *Scientific American* illustrates this point: the news features and background articles refer to mathematical models for such diverse problems as predicting the bunker-busting potential of nuclear warheads, evaluating the diffusion of ground toxins, describing the quantum state of nuclei, and understanding the emergence of complex patterns in evolution. Since most of the models developed for real applications are too difficult to solve analytically, scientists and engineers routinely use numerical simulation to investigate the behavior of the systems they study. The availability of sophisticated simulation techniques and increasingly powerful computers has contributed to the popularity of numerical simulation tools.

Although widely used, numerical simulation has its limitations. First of all, in order to derive predictions from the models, we need numerical values for the parameters and initial conditions. In many situations, especially outside the traditional science and engineering domains, such values are not available. In biochemistry, for example, reliable values for the kinetic parameters describing the rates of cellular reactions are usually difficult, if not impossible, to obtain with current experimental methods. The available information is usually qualitative in nature, such as that a reaction is fast or slow. Second, we are often not interested in the behavior of the system exhibited for particular values of the parameters and initial conditions. Rather, we would like to know which classes of qualitatively-different behaviors are compatible with the structure of the system, given certain constraints on the values of the parameters and initial conditions. For instance, when diagnosing a malfunctioning pump, it is important to know whether the assumption of a leaking pipe can explain the observation that the water pressure is lower than normal. In many cases, such qualitative predictions are sufficient for fault localization.

Human reasoning about the physical world often involves making qualitative predictions of the type described above. This is true for the common-sense reasoning that enables most people to infer what happens when an open bathtub is filled at a constant rate. But experts in medical physiology and electronic circuit design, to give but two examples, also demonstrate a qualitative understanding of their subject, resembling the common-sense reasoning of laymen in many aspects. The efficacy of human reasoning about physical mechanisms has inspired the development of *qualitative simulation* methods that address the limitations of traditional numerical methods. Early work on qualitative simulation explicitly mentioned human reasoning as its reference, defining the aims 'formalizing common-sense reasoning' or 'doing qualitative physics' (e.g. de Kleer, 1977; Forbus, 1983; Kuipers & Kassirer, 1984; Hayes, 1985). In subsequent work, this cognitive inspiration has gradually receded to the background, giving way to increased concerns about mathematical foundations.

A variety of qualitative simulation methods have been developed in the field of *qualitative reasoning (QR)*. Three what might be called classical approaches have emerged: the component-based approach of de Kleer and Brown (de Kleer & Bobrow, 1984; de Kleer & Brown, 1984, see also Williams, 1984b), the process-based approach of Forbus (Forbus, 1984; Forbus & de Kleer, 1993), and the constraint-based approach of Kuipers (1986, 1989a, 1994). The issues raised by these approaches have to a large extent shaped the work on qualitative simulation, and on qualitative reasoning more generally, up to this day (see Bobrow (1985) and Weld & de Kleer (1990) for collections of papers at the origin of the above methods, and Williams & de Kleer (1991), Forbus (1993) and Kuipers (1993a, b) for retrospectives).

In the ENVISION approach of de Kleer and Brown (de Kleer & Bobrow, 1984; de Kleer & Brown, 1984), a qualitative model of a system is constructed from the models of its individual components. This model takes the form of a set of confluences, i.e. constraints on the qualitative value (sign) of system variables. The confluences are used to infer a description of the behavior of the system through simulation. This results in an envisionment, a graph of all qualitative states of the system satisfying the confluences, and all possible transitions between these states. The *qualitative process theory (QPT)* approach developed by Forbus (Forbus, 1984; Forbus & de Kleer, 1993) provides a process-centered view on the physical world which allows one to express common-sense knowledge about physical systems. Given a scenario of a particular situation and a knowledge base of abstract model fragments describing objects, quantities, relations between objects, and processes in the domain, QPT generates a model of the physical system under study. The model is basically a set of constraints on the qualitative values of variables, called influences. As in the ENVISION approach, qualitative simulation is used to construct an envisionment describing the possible behaviors of the system. Unlike ENVISION and QPT, Kuipers' *qualitative simulation (QSIM)* approach Kuipers (1986, 1989a, 1994) has focused on the simulation process and, at least in its original formulation, has ignored the model-building aspect of qualitative reasoning. The qualitative model of a system takes the form of a qualitative differential equation, an abstraction of a class of ordinary differential equations. Qualitative simulation exploits continuity properties of the variables as well as constraints on their qualitative value implied by the qualitative differential equation. It produces possible sequences of qualitative states of the system, so-called qualitative behaviors.

Of the three approaches mentioned above, QSIM has become the most widely-used method for qualitative simulation. Its clear definition of concepts like qualitative model, qualitative state, and behavior, and its explicit relation between qualitative and numerical simulation, have facilitated the adaptation and integration of results from branches of mathematics dealing with ordinary differential equations. In addition, it has allowed the provision of guarantees on the validity of the outcome of the simulation process. On the other hand, ENVISION and QPT have exerted much influence on automated model building. The component-centered approach of ENVISION has inspired model-building approaches based on work in system dynamics, such as bond graphs (Karnopp *et al.*, 1990; Biswas & Yu, 1993; Borst *et al.*, 1997; Mosterman & Biswas, 2000). As a further contribution of ENVISION, one can cite the efforts to formulate a qualitative algebra, based on sign abstractions of real numbers. This has culminated in axiomatizations like the sign-real algebra of Williams (1984a, 1991) and the order-of-magnitude calculus of Raiman (1991). The process-centered ontology of QPT lies at the root of a number of model composition techniques (e.g. Falkenhainer & Forbus, 1991; Low & Iwasaki, 1992; Farquhar, 1994; Nayak, 1995; Levy *et al.*, 1997; Rickel & Porter, 1997), reviewed in Schut & Bredeweg, 1996; Xia & Smith, 1996; Keppens & Shen, 2001).

Over the years, the QR community has improved, generalized, and extended the above qualitative simulation methods as well as a large number of other methods (see Weld & de Kleer (1990) and Faltings & Struss (1992) for collections of papers, as well as the proceedings of the annual *International Workshop on Qualitative Reasoning*). Computer implementations of the methods have been developed and used in a variety of applications, including model-based diagnosis, design, automated modeling, machine learning, system identification, measurement analysis, and tutoring. Although at first restricted to traditional science and engineering domains, like classical mechanics and electrical engineering, applications in a wide variety of domains now exist. Many of the recent applications derive from domains where the difficulties in applying numerical methods are especially felt, such as medicine, biology, and ecology.

After the initial heydays in the 1980s and early 1990s, the interest in qualitative simulation has subsided a bit. The application of qualitative simulation to real-world problems has revealed some fundamental problems hampering existing methods. First of all, it was found that the predictions obtained through qualitative simulation may be weak and uninformative from a mathematical point of view. Moreover, it turned out to be difficult to scale up the methods, due to the explosion of the number of predicted behaviors when dealing with large and complex systems. In the course of time, a number of alternative approaches have emerged that, while preserving valuable ideas from qualitative simulation, integrate concepts and techniques from other fields in mathematics and computer science, in particular dynamic systems theory, control theory, and interval analysis. By tailoring the method to classes of dynamic systems for which strong mathematical constraints exist, or by taking into account (semi-)quantitative information, these *qualitative phase-space analysis* and *semi-quantitative simulation* approaches have been shown able to improve upon the results obtained with qualitative simulation.

The aim of this report is to review the classical qualitative simulation methods and diagnose the problems they have encountered. This assessment is followed by a discussion of the qualitative phase-space analysis and semi-quantitative simulation approaches, explaining how and to what extent they resolve these problems. It builds upon earlier reviews on qualitative simulation, such as the chapter introductions in Weld & de Kleer (1990), Kuipers' QSIM book (1994), recent book chapters by Forbus and Kuipers (Forbus, 1996; Kuipers, 2001), and an extensive review on qualitative reasoning by a French author collective (Dague & MQ&D, 1995) (see also Forbus, 1988; Fishwick & Luker, 1991; Kuipers, 1989a; de Kleer, 1992; Bredeweg & Struss, 2003). An excellent review placing qualitative simulation in the wider context of model-based reasoning is available in German (Struss, 2000). A new edition of a French textbook on qualitative reasoning (Travé-Massuyès & Dague, 2003), with chapters on many of the topics discussed in this report, recently appeared. The critical discussion of qualitative simulation by Sacks and Doyle (Sacks & Doyle, 1992) has also influenced the thrust of this review.

In Section 2, an overview of qualitative simulation methods will be given. Although the focus will be on QSIM, much of what is said about this method carries over to ENVISION and QPT. Being the technically most-developed qualitative simulation method, QSIM has integrated many ideas originating in the other methods in the course of time. Section 3 summarizes two classes of problems confronting QSIM and its relatives, preparing the introduction of the qualitative phase-space analysis and semi-quantitative simulation approaches in Sections 4 and 5, respectively.

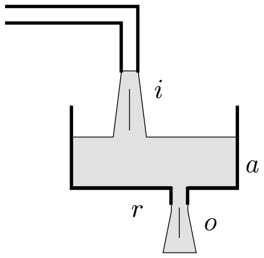


Figure 1 Simple tank system. The variables have the following interpretation: a water amount, r area of orifice, i inflow, o outflow. r and i are constants

The review finishes with a discussion of perspectives for qualitative simulation, arguing for a synthesis of the above-mentioned approaches.

2 Qualitative simulation: the QSIM method

The basic concepts and algorithms of QSIM will be illustrated by means of the simple tank system in Figure 1. Water flows into the tank at a (constant) rate i. The outflow of water from the tank is determined by the amount a of water in the tank and the area r of the orifice of the tank. The following differential equation model describes the behavior of the system:

$$\dot{a} = i - f(a,\ r), f \in\ M^{++}. \tag{1}$$

The function f is incompletely specified, in the sense that we only know that the outflow rate increases as the amount of water in the tank increases ($\partial f/\partial a > 0$) and as the area of the orifice increases ($\partial f/\partial r > 0$), here abbreviated to $f \in M^{++}$ (see Section 2.2 for the formal definition of M^{++}).

We will first explain how the behavior of the system can be described in a qualitative way (Section 2.1), followed by the abstraction of a qualitative model from an ordinary differential equation (Section 2.2). The possible qualitative behaviors of the system, consisting of sequences of qualitative states and transitions between qualitative states, are computed from the constraints on the qualitative values imposed by the model and the assumed continuity of the variables and their derivatives (Section 2.3). The QSIM algorithm and its correctness properties are discussed in Sections 2.4 and 2.5, respectively. The description of QSIM closely follows the original article (Kuipers, 1986) and the textbook (Kuipers, 1994). For more details the reader is referred to these sources.

2.1 Qualitative values, states, and behaviors

QSIM considers the variables $\boldsymbol{v}:[a,\ b] \to \mathbb{R}^{*m}$ of a dynamic system, where $\boldsymbol{v} = [v_1, \ldots, v_m]'$, $a,\ b \in \mathbb{R}$, and $\mathbb{R}^*$ represents the extended set of real numbers including ∞ and $-\infty$. The variables are considered to be *reasonable* functions of time, which among other things guarantees that they are continuously differentiable.

The possible qualitative values that a variable can take are determined by its *quantity space*. The quantity space is a total ordering of *landmark values* $l_1 < \ldots < l_k$. Each landmark value, or landmark for short, represents a usually unknown value in $\mathbb{R}^*$ that captures a qualitatively important distinction for the variable. For instance, the quantity space for the area r of the orifice in the tank example can be defined to contain the landmarks 0, *max*, and ∞, with $0 < max < \infty$. In the course of the simulation process, QSIM may introduce new landmark values (Kuipers, 1994). $-\infty$, 0, and ∞ are landmarks which by definition map to known values on the extended real line. The *sign quantity space* consists of these three landmarks. Time is itself a variable with the quantity space $t_0 < \ldots < t_n < \infty$. A time-point t is a *distinguished* time-point if a variable changes from or to a landmark value at t.

The *qualitative value of a variable v at time-point t* is expressed in terms of the landmarks in its quantity space and the direction of change. More specifically, the qualitative value of $v(t)$, $QV(v, t)$, with respect to the quantity space $l_1 < \ldots < l_k$, is the tuple $<qmag, qdir>$, where

$$qmag = \begin{cases} l_j & \text{if } v(t) = l_j, \\ ]l_j, l_{j+1}[& \text{if } l_j < v(t) < l_{j+1}, \end{cases} \quad \text{and} \quad qdir = \begin{cases} inc & \text{if } \dot{v}(t) > 0, \\ std & \text{if } \dot{v}(t) = 0, \\ dec & \text{if } \dot{v}(t) < 0. \end{cases}$$

qmag and *qdir* are called the *qualitative magnitude* and *qualitative direction*, respectively, of v at t. For example, the area r of the orifice at t_0 is represented by the qualitative value $QV(r, t_0) = <max, std>$. Since r is a constant, it will have the same qualitative value at a later time-point: $QV(r, t_1) = <max, std>$. If the orifice is only partially opened, then the qualitative value of its area, $QV(r, t_0)$, equals $<]0\ max[, std>$ (*idem* for later time-points).

The *qualitative value of a variable v on a time-interval* $]t_i, t_{i+1}[$, where t_1 and t_{i+1} are adjacent distinguished time-points, follows from the qualitative value at the time-points in the interval. In particular, the qualitative value of v on $]t_i, t_{i+1}[$, $QV(v, t_i, t_{i+1})$, is defined to be equal to $QV(v, t)$ for any $t \in]t_i, t_{i+1}[$. Since t_i and t_{i+1} are adjacent distinguished time-points, this qualitative value is unique. If the tank is filled from empty, then between the initial time-point t_0 and the next distinguished time-point t_1 the tank will contain a positive and increasing amount of water, more particularly $QV(a, t_0, t_1) = <]0, \infty[, inc>$.

A *qualitative state* of a dynamic system at a distinguished time-point or on an interval between two adjacent distinguished time-points is an m-tuple of qualitative values, one for each variable in $\boldsymbol{v}$:

$$QS(\boldsymbol{v}, t_i) = <QV(v_1, t_i), \ldots, QV(v_m, t_i),>$$
$$QS(\boldsymbol{v}, t_i, t_{i+1}) = <QV(v_1, t_i), t_{i+1}, \ldots, QV(v_m, t_i, t_{i+1})>,$$

where t_i and t_{i+1} are distinguished time-points of some of the variables in $\boldsymbol{v}$.

The *qualitative behavior* of a dynamic system on $[a, b]$ is the sequence of qualitative states

$$QB(\boldsymbol{v}) = <QS(\boldsymbol{v}, t_0), QS(\boldsymbol{v}, t_0, t_1), QS(\boldsymbol{v}, t_1), \ldots, QS(\boldsymbol{v}, t_{p-1}, t_p), QS(\boldsymbol{v}, t_p)>,$$

with $t_0 = a$ and $t_p = b$. Notice that the sequence alternates between time-point and time-interval states. According to the *behavior abstraction* theorem of QSIM, such a qualitative behavior can be uniquely abstracted for each vector $\boldsymbol{v}$ of reasonable functions. The functions $\boldsymbol{v}$ are said to be *consistent with* or to *satisfy* the qualitative behavior. Conversely, a qualitative behavior will usually be satisfied by a class of reasonable functions.

2.2 Qualitative differential equations

QSIM models dynamic systems by means of *qualitative differential equations (QDEs)*. A QDE is an abstraction of an ordinary differential equation (ODE), usually written in the form of a system of n coupled equations

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{p}), \tag{2}$$

where $\boldsymbol{x} = [x_1, \ldots, x_n]'$ is the vector of state variables and $\boldsymbol{p} = [p_1, \ldots, p_k]'$ the parameter vector. The functions $\boldsymbol{f} = [f_1, \ldots, f_n]'$, with $f_i : \Omega \to \mathbb{R}^*$, $1 \le i \le n$, are assumed to be continuously differentiable inside a closed region $\Omega \subseteq \mathbb{R}^{*n}$ in which the ODE is defined, the *operating region*.

The right-hand side of (2) is composed of functions that may be incompletely specified, in the sense that they are only known to belong to a certain monotonicity class. Kuipers (1994) lists a number of such monotonicity classes. M^+ is the class of monotonically increasing functions, that

Table 1 Qualitative constraints and the basic mathematical equations of which they are abstractions

Qualitative constraints	Basic equations
EQUAL (x, y)	$y(t)=x(t)$
ADD (x, y, z)	$z(t)=y(t)+x(t)$
MULT (x, y, z)	$z(t)=y(t)\times x(t)$
MINUS (x, y)	$y(t)=-x(t)$
D/DT (x, y)	$\dot{y}(t)=x(t)$
CONSTANT (x)	$\dot{x}(t)=0$
M^+ (x, y)	$y(t)=f(x(t)), f \in M^+$
M_0^+ (x, y)	$y(t)=f(x(t)), f \in M_0^+$
M^{++} (x, y, z)	$z(t)=f(y(t), x(t)), f \in M{+}{+}$

Analogous constraints for subtraction (−), division (/), monotonically decreasing functions (M^-, M_0^-), and other multivariate monotonic functions (M^{--}, M^{+-}, M^{-+}) have been omitted.

(a)		(b)
$i:$	$0 < \infty$	D/DT(n, a)
$a:$	$0 < full < \infty$	ADD(n, o, i)
$o:$	$0 < \infty$	$M^{++}(a, r, o)$
$n:$	$-\infty < 0 < \infty$	CONSTANT(i)
$r:$	$0 < max < \infty$	CONSTANT(r)

Figure 2 QDE abstracted from the ODE model describing the tank system of Figure 1: (a) quantity spaces of the variables and (b) qualitative constraints

is, for every $f \in M^+$ and $y=f(x)$ it holds that $df/dx>0$ over the domain of the function. Similarly, M^- is the class of monotonically decreasing functions. M_0^+ and M_0^- are the classes of monotonically increasing and decreasing functions, respectively, such that for every function f in these classes, we have $f(0)=0$. The monotonicity classes can be generalized to multivariate functions in an obvious manner. For instance, M^{++} is the class of functions f, with $z=f(x, y)$, such that $\partial f/\partial x>0$ and $\partial f/\partial y>0$ over the domain.

Formally, a QDE consists of a set of constraints on the system variables, so-called *qualitative constraints*. A QDE is abstracted from an ODE by first decomposing the latter into a set of basic mathematical equations, and then mapping the equations to the corresponding qualitative constraints (Table 1). The system variables, denoted by $\mathbf{v}$, include the state variables $\mathbf{x}$ and the parameters $\mathbf{p}$, but also any auxiliary variables introduced through the reduction of the ODE to basic equations.

Consider the ODE model describing the tank system in Figure 1. The differential equation $\dot{a}=i-f(a, r), f \in M^{++}$, can be translated into the basic equations $\dot{a}=n$, $i=n+o$, and $o=f(a, r)$, where n and o are auxiliary variables representing the net flow and the outflow of the tank. The corresponding qualitative constraints are D/DT(n, a), ADD(n, o, i), and $M^{++}(a, r, o)$. Adding the quantity spaces for the variables, we obtain the QDE shown in Figure 2.

The *structural abstraction* theorem of QSIM states that each ODE can be abstracted into a QDE, such that any solution $\boldsymbol{v}:[a, b]\rightarrow\mathbb{R}^{*m}$ of the ODE is consistent with the constraints of the QDE. The structural abstraction theorem does not imply that the QDE is obtained by abstraction from some previously-known ODE, as in the example. Most of the time, such an ODE does not exist and the QDE has to be directly specified from the available qualitative information. However, formally speaking, this QDE is an abstraction of an ODE, or more precisely, of a class of ODEs, which provides the basis of the correctness properties of the simulation algorithm (Section 2.5).

Table 2 Definition of the ADD constraint

	$qmag_z$	$qmag_y$: $]-\infty, 0[$	$qmag_y$: 0	$qmag_y$: $]0, \infty[$
$qmag_x$	$]-\infty, 0[$	$]-\infty, 0[$	$]-\infty, 0[$	?
	0	$]-\infty, 0[$	0	$]0, \infty[$
	$]0, \infty[$	?	$]0, \infty[$	$]0, \infty[$

	$qdir_z$	$qdir_y$: *dec*	$qdir_y$: *std*	$qdir_y$: *inc*
$qdir_x$	*dec*	*dec*	*dec*	?
	std	*dec*	*std*	*inc*
	inc	?	*inc*	*inc*

A question mark means that the qualitative magnitude (direction) of z can be any of $]-\infty, 0[$, 0, and $]0, \infty[$ (*dec, std*, and *inc*).

2.3 Constraints on qualitative values

The solutions of the ODEs satisfying a QDE usually correspond to different qualitative behaviors. How are these behaviors computed? Three types of constraint are used to determine qualitative states and transitions between qualitative states: state constraints (Section 2.3.1), transition constraints (Section 2.3.2), and global constraints (Section 2.3.3).

2.3.1 State constraints

The first type of constraint puts restrictions on the qualitative values of variables in a qualitative state $QS(t_i)$ or $QS(t_i, t_{i+1})$. These are the qualitative constraints making up a QDE, also called *state constraints*. Given an incompletely-specified qualitative state, consisting of qualitative values for only some of the variables, the state constraints dictate which alternative completions are possible. Each qualitative constraint in Table 1 constrains the qualitative magnitude and direction of the variables involved. This will be illustrated below for two examples, assuming that the variables take their value from the sign quantity space discussed above. The validity of the constraints can be easily demonstrated by referring to the mathematical equations from which they have been abstracted.

Consider the qualitative constraint ADD(x, y, z). This constraint determines which qualitative values $<qmag_x, qdir_x>$, $<qmag_y, qdir_y>$, and $<qmag_z, qdir_z>$ of the variables x, y, and z are permitted. Assuming that the magnitudes of x, y, and z are finite, the ADD constraint is defined in Table 2. The definition of ADD implies, for instance, that if $qval_x = <]0, \infty[, inc>$ and $qval_y = <0, std>$, then necessarily $qval_z = <]0, \infty[, inc>$.

The qualitative constraint M+(x, y) implied by $y = f(x)$, $f \in M^+$, is defined as $qdir_x = qdir_y$. There are no constraints on the qualitative magnitudes, since the point at which f crosses the x-axis is not known. If f were an element of M_0^+, then we would additionally have $qmag_x = qmag_y$.

Notice that the use of qualitative information may lead to ambiguities. Given that ADD(x, y, z), $qmag_x =]-\infty, 0[$, and $qmag_y =]0, \infty[$, the qualitative magnitude of z can take any sign. The ADD constraint does not rule out any of these alternatives, since all of them are consistent with the qualitative information. During state completion the occurrence of ambiguities causes the simulation algorithm to produce several qualitative states consistent with the constraints (Section 2.4).

The variables in the system may have other quantity spaces than the sign quantity space. The above constraints remain valid in the general case, but can be refined if *corresponding values* are taken into account. Corresponding values are tuples of landmark values for which a certain equation is satisfied.[1] For instance, let l_x, l_y, and l_z be landmark values for x, y, and z, respectively, such that $-\infty < 0 < l_x < \infty$, $-\infty < 0 < l_y < \infty$, and $-\infty < 0 < l_z < \infty$. Suppose that $<l_x, l_y, l_z>$ is a corresponding-value triple for the ADD constraint. If $qmag_x =]l_x, \infty[$ and $qmag_y = l_y$, then we can immediately infer

[1] For a generalization of the definition of corresponding values, based on the use of intervals with landmark value bounds, see Say & Kuru (1993).

Table 3 Constraints on transitions from a qualitative state to successor qualitative states

P-transitions		I-transitions	
$QV(v, t_i)$ $\Rightarrow$	$QV(v, t_i, t_{i+1})$	$QV(v, t_i, t_{i+1})$ $\Rightarrow$	$QV(v, t_{i+1})$
$<l_j, std>$	$<l_j, std>$	$<l_j, std>$	$<l_j, std>$
$<l_j, std>$	$<]l_j, l_{j+1}[, inc>$	$<]l_j, l_{j+1}[, inc>$	$<l_{j+1}, std>$
$<l_j, std>$	$<]l_{j-1}, l_j[, dec>$	$<]l_j, l_{j+1}[, inc>$	$<l_{j+1}, inc>$
$<l_j, inc>$	$<]l_j, l_{j+1}[, inc>$	$<]l_j, l_{j+1}[, inc>$	$<]l_j, l_{j+1}[, inc>$
$<l_j, dec>$	$<]l_{j-1}, l_j[, dec>$	$<]l_j, l_{j+1}[, inc>$	$<]l_j, l_{j+1}[, std>$
$<]l_j, l_{j+1}[, inc>$	$<]l_j, l_{j+1}[, inc>$	$<]l_j, l_{j+1}[, dec>$	$<l_j, std>$
$<]l_j, l_{j+1}[, dec>$	$<]l_j, l_{j+1}[, dec>$	$<]l_j, l_{j+1}[, dec>$	$<l_j, dec>$
$<]l_j, l_{j+1}[, std>$	$<]l_j, l_{j+1}[, std>$	$<]l_j, l_{j+1}[, dec>$	$<]l_j, l_{j+1}[, dec>$
$<]l_j, l_{j+1}[, std>$	$<]l_j, l_{j+1}[, inc>$	$<]l_j, l_{j+1}[, dec>$	$<]l_j, l_{j+1}[, std>$
$<]l_j, l_{j+1}[, std>$	$<]l_j, l_{j+1}[, dec>$	$<]l_j, l_{j+1}[, std>$	$<]l_j, l_{j+1}[, std>$

P-transitions are transitions from a time-point to a time-interval, while I-transitions are transitions from a time-interval to a time-point.

that $qmag_z =]l_z, \infty[$. In order to formalize the state constraints in an appropriate and general way, Kuipers (1994) uses the sign-real algebra of Williams (1991).

2.3.2 *Transition constraints*

A qualitative behavior consists of a sequence of qualitative states, alternating between states coinciding with a time-point and states lasting over a time-interval. The second type of constraint imposes restrictions on the *transitions* from a particular time-point state $QS(t_i)$ to successor time-interval states $QS(t_i, t_{i+1})_1, \ldots, QS(t_i, t_{i+1})_s$, or from a time-interval state $QS(t_i, t_{i+1})$ to successor time-point states $QS(t_{i+1})_1, \ldots, QS(t_{i+1})_s$. These so-called *transition constraints* are based on the continuity properties of the variables and their derivatives. For continuously differentiable functions the intermediate-value and mean-value theorems from differential calculus (Spivak, 1967) allow only a few possible transitions from one qualitative value to another. For instance, the qualitative magnitude of a variable cannot change from positive to negative without passing through 0. The transition constraints rule out candidate successor states whose variables have qualitative values that are not consistent with these restrictions.

Two kinds of transition are distinguished in QSIM: transitions from a time-point to a time-interval (*point transitions* or *P-transitions*) and transitions from a time-interval to a time-point (*interval transitions* or *I-transitions*). Table 3 summarizes the possible successor relations for a continuously differentiable function $v:[a, b] \rightarrow \mathbb{R}^*$, where $l_{j-1} < l_j < l_{j+1}$ are three adjacent landmarks in the quantity space of v.

2.3.3 *Global constraints*

The qualitative constraints discussed so far are local, in the sense that they pertain to a single qualitative state or to a pair of successive qualitative states. The locality of the analysis may lead QSIM to generate qualitative states which are not valid in the light of the sequence of qualitative states preceding it. In order to filter out these qualitative states, a third type of constraint can be formulated which puts restrictions on sequences of qualitative states. In Section 3.1, such *global constraints* will be discussed in more detail.

2.4 *Qualitative simulation algorithm*

The basic idea underlying qualitative simulation is often schematically summarized by means of Figure 3. The aim of qualitative simulation is to generate from a QDE and initial qualitative state

$$\begin{tikzcd}
\text{Qualitative differential equation (QDE)} \arrow[r, "\text{qualitative simulation}"] & \text{Qualitative behavior} \\
\text{Ordinary differential equation (ODE)} \arrow[u, "\text{abstraction}"'] \arrow[r, "\text{analytical solution or}", "\text{numerical simulation}"'] & \boldsymbol{v} \,:\, [a, b] \to \mathbb{R}^{*m} \arrow[u, "\text{abstraction}"']
\end{tikzcd}$$

Figure 3 Abstraction relations in qualitative simulation

information QS_{init} those qualitative behaviors that are abstractions of the solutions of the class of ODEs satisfying the QDE. The algorithm starts by completing the initial state information to all qualitative states consistent with the state constraints. Next, it determines for each completed state its possible successors, using the transition constraints. The successor states consistent with the state constraints and global constraints are linked to the completed initial state. This procedure of successor generation is recursively applied to the successor states, except if such a state:

1. is a *quiescent* state, that is, a state in which all variables have a qualitative direction equal to *std*;
2. is a *transition state*, that is, included in the boundary of the operating region and moving outward;
3. is identical to a previous state, indicating a cyclic qualitative behavior; or
4. occurs at $t = \infty$.

For each completed initial state, the simulation algorithm thus produces a *qualitative behavior tree*. The qualitative behaviors are the paths from the root(s) to the leafs of a tree, that is, from the initial state(s) to states without successors. Given a QDE with variables **v** and initial qualitative state information $QS(init)$, the following algorithm formally describes the generation of qualitative behavior trees in QSIM.

Step 1 Complete $QS(init)$ to initial states $QS(t_0)_1, \ldots, QS(t_0)_s$, which are the roots of the behavior trees. Put the completed initial states on the agenda.

Step 2 If the agenda is empty, then stop; the paths from the roots to the leafs in the behavior trees are the qualitative behaviors $QB_1, \ldots, QB_l$. Otherwise, pop a state $QS(t_i)$ or $QS(t_i, t_{i+1})$ from the agenda.

Step 3 For each variable v of the system, use the transition constraints to determine the possible successors of $QS(t_i)$ or $QS(t_i, t_{i+1})$.

Step 4 Determine the successor states consistent with the state constraints and global constraints. Add these states to the behavior tree by linking them to $QS(t_i)$ or $QS(t_i, t_{i+1})$.

Step 5 Add each eligible successor state to the agenda. A successor state is eligible, unless it is quiescent, identical to a previous state, a transition state, or occurring at $t = \infty$. Continue with step 2.

The above description of the QSIM algorithm concentrates on its basic features; it leaves out details and attempts a rational reconstruction of some aspects. For instance, the source references describe how state completion in steps 1 and 4 of the algorithm is achieved by formalizing it as a constraint satisfaction problem (CSP). QSIM uses the algorithm Cfilter (Kuipers, 1994) for efficiently solving this CSP. Most global constraints are applied only after the states have been completed by Cfilter and added to the behavior tree.

At a *transition state* the boundary of an operating region is reached and transgressed. If there is a model for the system in the region which QSIM is about to enter, qualitative simulation can be resumed in the new region with initial state(s) defined by a *transition function*. The variables may be discontinuous across region transitions.

The QSIM algorithm has been implemented in a computer program for the qualitative simulation of systems described by QDEs (Farquhar *et al.*, 1993). The qualitative behaviors resulting from the simulation process can be analyzed and graphically displayed. The user has the opportunity to control the simulation by switching on and off filters that check consistency of the states with the various types of constraint. A trace facility allows one to observe the impact of different constraints in the simulation process and debug the models. The implementation of QSIM has been written in Common Lisp and is available at `http://www.cs.utexas.edu/users/qr/`.[2]

The behavior of a tank system filled from empty can be simulated by means of QSIM, using the following initial state information:

$$QS(init)=<QV(a,\ t_0)=<0,\ \_>,\ QV(i,\ t_0)=<]0,\infty[,\ std>,\ QV(r,\ t_0)=<]0,\ max[,\ std>>,$$

where _ means that the value is unspecified. The initial state information is completed into a single initial qualitative state by inferring that the qualitative direction of a at t_0 is *inc* (step 1). This state is popped from the agenda in step 2. Using the constraints, a single successor state on $]t_0, t_1[$ is generated (steps 3 and 4). Adding this state to the agenda (step 5), and repeating steps 2–4, yields three successor states at t_1. None of these states is eligible (step 5), so the simulation finishes at step 2 in the next pass of the loop.

The qualitative behavior tree resulting from the simulation is shown in Figure 4(a). Two of the three behaviors are detailed in parts (b) and (c) of the figure. In the first behavior, shown in (b), the amount of water continues to increase until the tank is full and a transition state is reached (the tank overflows). In the second behavior, the tank reaches equilibrium at the very moment when the tank is full, while in the third behavior, shown in (c), equilibrium is reached before the tank is full. Notice that, contrary to numerical simulation, several possible behaviors of the system are predicted in the example. The available qualitative information is not sufficiently constraining to determine whether the net flow reaches the landmark 0 before, after, or at the same time when the amount of water reaches the landmark *full*.

2.5 Properties of qualitative simulation

A productive way to look at QSIM (Kuipers, 1993a) is to view it as a theorem prover deriving theorems of the following form:

$$\text{QSIM} \vdash QDE \wedge QS(init) \rightarrow QB_1 \vee \ldots \vee QB_l.$$

QSIM proves from a QDE and initial qualitative state information $QS(init)$ the disjunction of qualitative behaviors $QB_1 \vee \ldots \vee QB_l$. Intuitively, this could be interpreted as follows: the solution of any initial-value problem $ODE \wedge \mathbf{v}(t_0)=\mathbf{v_0}$ satisfying $QDE \wedge QS(init)$ is described by some qualitative behavior in $QB_1 \vee \ldots \vee QB_l$. The disjunction may contain *spurious* qualitative behaviors, that is, behaviors which describe no solution to any initial-value problem satisfying the QDE and initial qualitative state information. A well-known example of a spurious qualitative behavior is the mass-spring behavior violating the law of energy conservation (Kuipers, 1994), which will be discussed in Section 3.1. Notwithstanding the occurrence of spurious qualitative behaviors, the disjunction $QB_1 \vee \ldots \vee QB_l$ is guaranteed to contain all non-spurious or *genuine* behaviors of the system. As a consequence, the theorems derived by QSIM are always true, which explains why the method is called *sound*. However, if the disjunction includes spurious behaviors, QSIM fails to prove the stronger theorem *without* these behaviors. As a consequence, the method is called *incomplete*.[3]

An estimate of the complexity of the QSIM algorithm is given by the number of qualitative states that need to be generated. In the worst case, the number of successors of a qualitative state increases exponentially with the number of variables (Kuipers, 1986). What is more, the algorithm need not halt and can continue producing ever more and ever longer qualitative behaviors.

[2] Other implementations of QSIM, in Prolog and in C++, are described in Bandelj *et al.* (2002) and Eisenack & Petschel-Held (2002). For implementations of QPT, see Forbus (1989) and Forbus & de Kleer (1993).

[3] Although the above definitions of soundness and completeness have become standard in the field, they are not undisputed (Struss, 1988b).

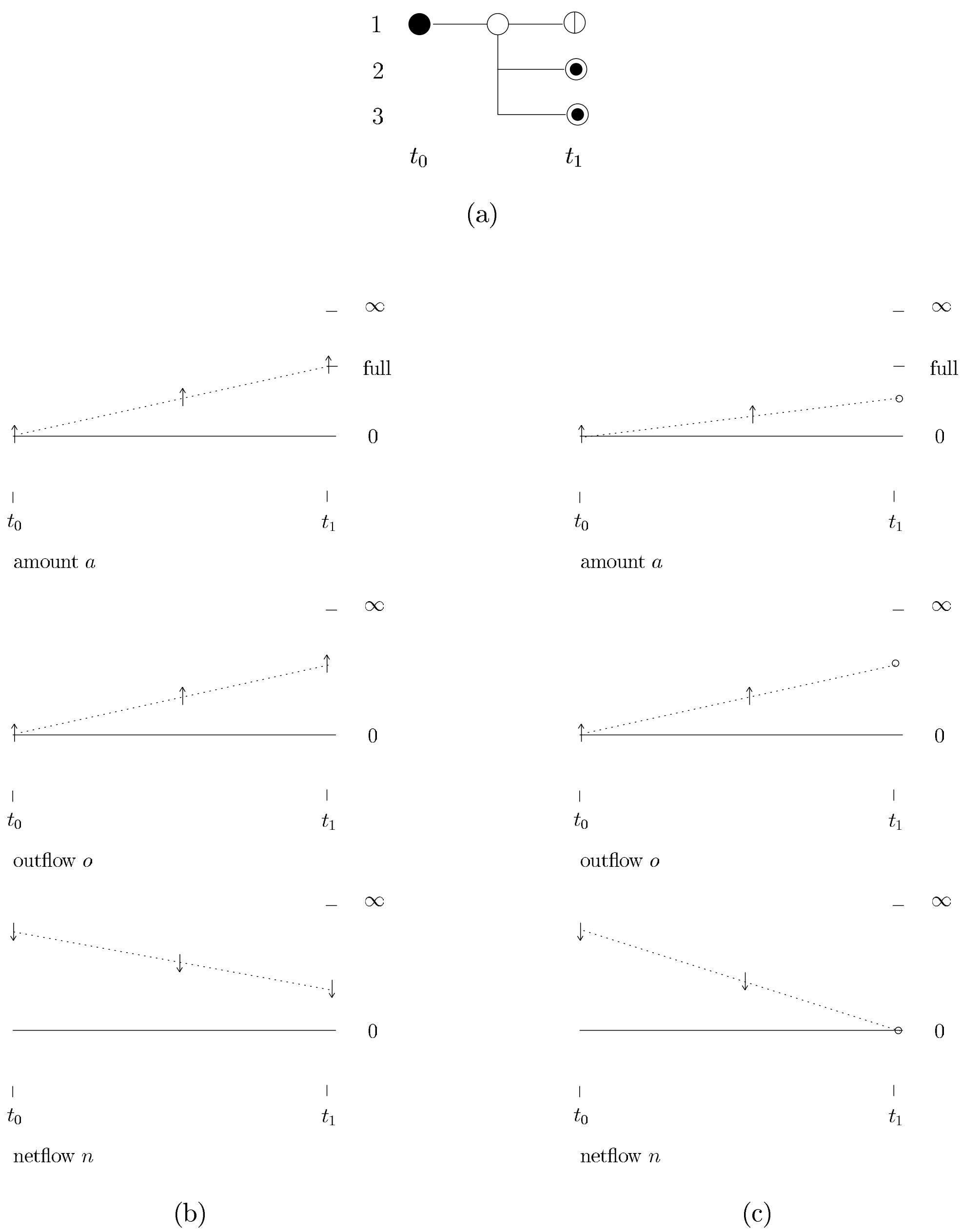


Figure 4 (a) Qualitative behavior tree for the simple tank system in Figure 1. (b)–(c) The temporal evolution of a few distinctive variables according to the qualitative behaviors 1 and 3. The notation is as follows: ● denotes a qualitative state at a time-point, ○ a qualitative state over a time-interval, ⦿ a quiescent state, ⦶ a transition state, and ◎ the end of a period. The symbols $\uparrow$, $\downarrow$, and $\circ$ in the plots refer to increasing, decreasing, and steady directions, respectively (Farquhar *et al.*, 1993)

3 Extensions of QSIM

In summary, qualitative simulation in the QSIM framework allows one to make predictions on the behavior of a system from qualitative models that are abstractions of ordinary differential equations. Instead of numerical values for the parameters, relations between symbolic values are used, while algebraic functions may be incompletely specified, that is, defined by their monotonicity properties only. The resulting qualitative behaviors are interpreted as abstractions of numerical solutions, capturing qualitative features of the solutions, such as the temporal ordering of maxima and minima of the variables.

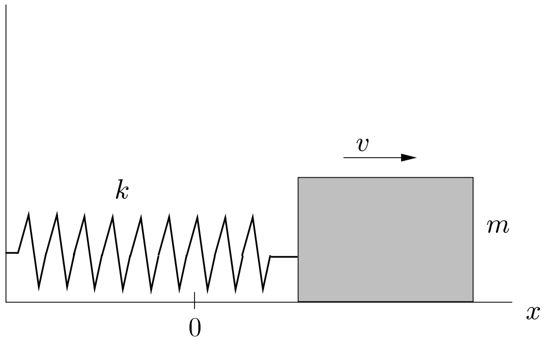


Figure 5 Undamped mass–spring system. The variables refer to the position x, velocity v, acceleration a, and mass m of the block, as well as the spring constant k

The basic idea of qualitative simulation, summarized in Figure 3, is intuitively plausible due to its analogies with numerical simulation. However, several problems often complicate the practical application of QSIM. In this section, two categories of problems will be discussed, the occurrence of spurious behaviors (Section 3.1) and the combinatorial explosion of behavior trees (Section 3.2), together with extensions of the basic algorithm to counter these problems. Although the technical details are different, the problems also occur in the other qualitative simulation methods mentioned in the introduction. The evaluation of the problems and extensions in Section 3.3 prepares the way for the discussion of qualitative phase-space analysis and semi-quantitative simulation approaches in the next two sections.

3.1 Spurious qualitative behaviors

The simulation algorithm of QSIM recursively generates qualitative states and transitions to successor states, as explained in Section 2.4. The qualitative behaviors in the resulting behavior tree may be spurious, in the sense that they do not correspond to any solution of an ODE of which the QDE is an abstraction. The occurrence of spurious qualitative behaviors can be traced back to the generation of spurious qualitative states, spurious transitions between qualitative states, or spurious sequences of qualitative states. In this section, examples of each of these causes will be given.

3.1.1 Spurious qualitative states

Consider the well-known undamped mass–spring system shown in Figure 5. The variable x describes the position of the mass with respect to the rest position. Assuming a unit mass, the spring force f_s is given by

$$f_s = -k(x - x^3), \tag{3}$$

with k denoting the spring constant ($k>0$). The equation expresses that the stiffness of the spring decreases with increasing displacement from the rest position.

Decomposing (3) into basic equations, and abstracting these into qualitative constraints, results in the model fragment shown in Figure 6(a). Notice that, for clarity of exposition, the expressions $-k$, $x - x^3$, x^3, and x^2 are used as names of auxiliary variables. Since 1 and -1 are roots of (3), in addition to 0, we add landmark values corresponding to these numbers to the quantity spaces of the variables. Furthermore, appropriate corresponding value triples are defined for the constraints (not shown).

What happens when the displacement is larger than 1, that is, when the qualitative magnitude of x equals $]1, \infty[$? The qualitative constraints in Figure 6(a) do not provide a unique value for the qualitative magnitude of f_s. A qualitative magnitude $]1, \infty[$ for x gives a qualitative magnitude $]1, \infty[$ for x^3, but this does not allow to decide on the sign of $x - x^3$, and hence on the sign of f_s. As

(a)	(b)
MULT$(-k, x - x^3, f_s)$	MULT$(-k, x - x^3, f_s)$
ADD$(x - x^3, x^3, x)$	MULT$(x, 1 - x^2, x - x^3)$
MULT(x^2, x, x^3)	ADD$(1 - x^2, x^2, 1)$
MULT(x, x, x^2)	MULT(x, x, x^2)
MINUS$(k, -k)$	MINUS$(k, -k)$
CONSTANT(k)	CONSTANT(k)
	CONSTANT(1)

Figure 6 (a) Set of qualitative constraints abstracted from the spring force equation $f_s = -k(x - x^3)$. (b) Alternative set of qualitative constraints obtained from the same equation

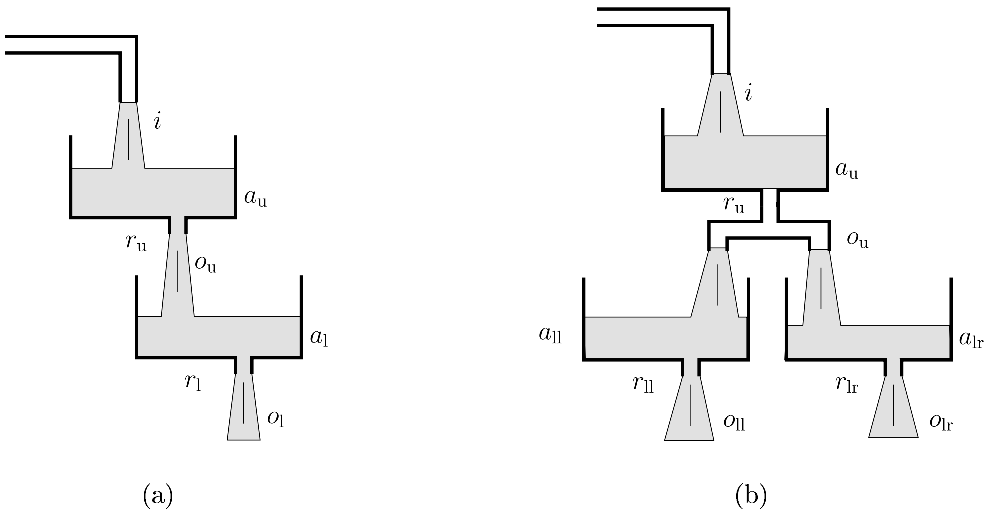


Figure 7 Two cascaded-tank systems. The variable names have the following interpretation: *a* water amount, *r* area of orifice, *i* inflow, *o* outflow. *r* and *i* are constants. The subscripts $\cdot_u$ and $\cdot_l$ refer to the upper and lower tanks, respectively, while $\cdot_{ll}$ and $\cdot_{lr}$ denote the lower-left and lower-right tank, respectively

a consequence, QSIM will generate several qualitative states, distinguishing between cases in which f_s has the qualitative magnitude $]-\infty, 0[$, 0,or $]0, \infty[$.

However, this result is not correct, since two of the three solutions can be shown to be spurious. In fact, $]0, \infty[$ is the only possible qualitative magnitude for f_s, which follows directly from the fact that x^3>x, if x>1. As a consequence of the abstraction of the original equation into a set of qualitative constraints, and the local nature of constraint processing by Cfilter, QSIM is not able to infer the correct result. This example is an instance of what is called the problem of *dependencies* in interval arithmetic, arising when a variable appears more than once in a set of equations (Moore (1979); see Struss (1988b) for a discussion in the context of QR). In some cases, the dependencies can be avoided by choosing a different decomposition of the original equation into basic equations. This is illustrated in Figure 6(b). The only possible qualitative magnitude for f_s is now found to be $]0, \infty[$, as desired.

3.1.2 Spurious transitions between qualitative states

Apart from the generation of spurious qualitative states, spurious behaviors may arise from spurious state transitions. As an example, consider the cascaded-tanks system in Figure 7(a). Water flows into the upper tank at a (constant) rate *i*. The outflow of water from the upper and lower tanks is determined by the amounts of water in the tanks (a_u and a_l, respectively) and the areas of the orifices of the tanks (r_u and r_l). The system is described by the following pair of equations:

$$\dot{a}_u = i - f(a_u, r_u),\ f \in M^{++},$$
$$\dot{a}_l = f(a_u, r_u) - g(a_l, r_l),\ g \in M^{++}.$$

The corresponding QDE model is shown in Figure 8. It contains auxiliary variables $n_u = i - o_u$ and $o_u = f(a_u, r_u)$ for the net flow and outflow of the upper tank. Similarly, $n_l = o_u - o_l$ and $o_l = g(a_l, r_l)$ denote the net flow and outflow of the lower tank.

Now suppose that we start at t_0 by filling the upper and lower tank from empty, while both orifices are maximally open: $QV(a_u, t_0) = \langle 0, \_ \rangle$, $QV(a_l, t_0) = \langle 0, \_ \rangle$ $QV(r_u, t_0) = \langle max, std \rangle$, $QV(r_l, t_0) = \langle max, std \rangle$, and $QV(i, t_0) = \langle]0, \infty[, std \rangle$. The state constraints determine a unique initial qualitative state, in which the net flow in the upper tank is decreasing and the net flow in the lower tank increasing: $QV(n_u, t_0) = \langle]0, \infty[, dec \rangle$ and $QV(n_u, t_0) = \langle]0, \infty[, inc \rangle$. The initial qualitative state has a unique successor state, in which the amounts of water in the upper and lower tank are increasing, that is, $QV(a_u, t_0, t_1) = \langle]0, \infty[, inc \rangle$ and $QV(a_l, t_0, t_1) = \langle]0, \infty[, inc \rangle$. In addition, $QV(n_u, t_0, t_1) = \langle]0, \infty[, dec$ and $QV(n_l, t_0, t_1) = \langle]0, \infty[, inc \rangle$. At t_1 the net flow into the lower tank reaches a maximum, $QV(n_l, t_1) = \langle]0, \infty[, std \rangle$, while $QV(n_u, t_1)$ has not changed with respect to $]t_0, t_1[$. Now what is the qualitative value of n_l immediately after t_1? The transition constraints in Table 3 permit three possibilities: $QV(n_l, t_1, t_2)$ can be $\langle]0, \infty[, dec \rangle$, $\langle]0, \infty[, std \rangle$, or $\langle]0, \infty[, inc \rangle$. None of these possibilities is excluded by the state constraints, so that QSIM generates three successors of the qualitative state at t_1.

Under certain conditions, some of these transitions are spurious. This can be seen by focusing on the sign of the second-order time derivative of n_l at t_1. If f and g are linear in a_u and a_l, respectively, we obtain:

$$\ddot{n}_l = \frac{\partial}{\partial a_u} f(a_u, r_u)\dot{n}_u - \frac{\partial}{\partial a_l} g(a_l, r_l)\dot{n}_l.$$

Bearing in mind that $f, g \in M^{++}$, and $\dot{n}_l = 0$ and $\dot{n}_u < 0$ at t_1, we infer that $\ddot{n}_l < 0$ at t_1. Because the second-order time derivative of n_l is negative when n_l reaches its critical point, it follows that $\dot{n}_l$ must be decreasing immediately afterwards. This leaves only a single successor state in the interval $]t_1, t_2[$, for which it holds that $QV(n_l, t_1, t_2) = \langle]0, \infty[, dec \rangle$.

QSIM has been extended to avoid spurious transitions caused by the ignoring of higher-order time derivatives. Kuipers and colleagues have proposed a special constraint applied in step 4 of the simulation algorithm discussed in Section 2.4 (Kuipers *et al.*, 1991; Kuipers, 1994). The constraint preserves soundness under the so-called *sign-equality assumption*, of which the linearity of f and g in the example is a special case. Hossain & Ray (1997) have generalized the qualitative state description and transition table to take into account second-order time derivatives. This work

i :	$0 < \infty$	D/DT(n_u, a_u)
a_u :	$0 < \infty$	ADD(n_u, o_u, i)
a_l :	$0 < \infty$	$M^{++}(a_u, r_u, o_u)$
o_u :	$0 < \infty$	D/DT(n_l, a_l)
o_l :	$0 < \infty$	ADD(n_l, o_l, o_u)
n_u :	$-\infty < 0 < \infty$	$M^{++}(a_l, r_l, o_l)$
n_l :	$-\infty < 0 < \infty$	CONSTANT(i)
r_u :	$0 < max < \infty$	CONSTANT(r_u)
r_l :	$0 < max < \infty$	CONSTANT(r_l)
	(a)	(b)

Figure 8 QDE abstracted from the ODE describing the cascaded-tank system of Figure 7(a): (a) quantity spaces of variables and (b) qualitative constraints

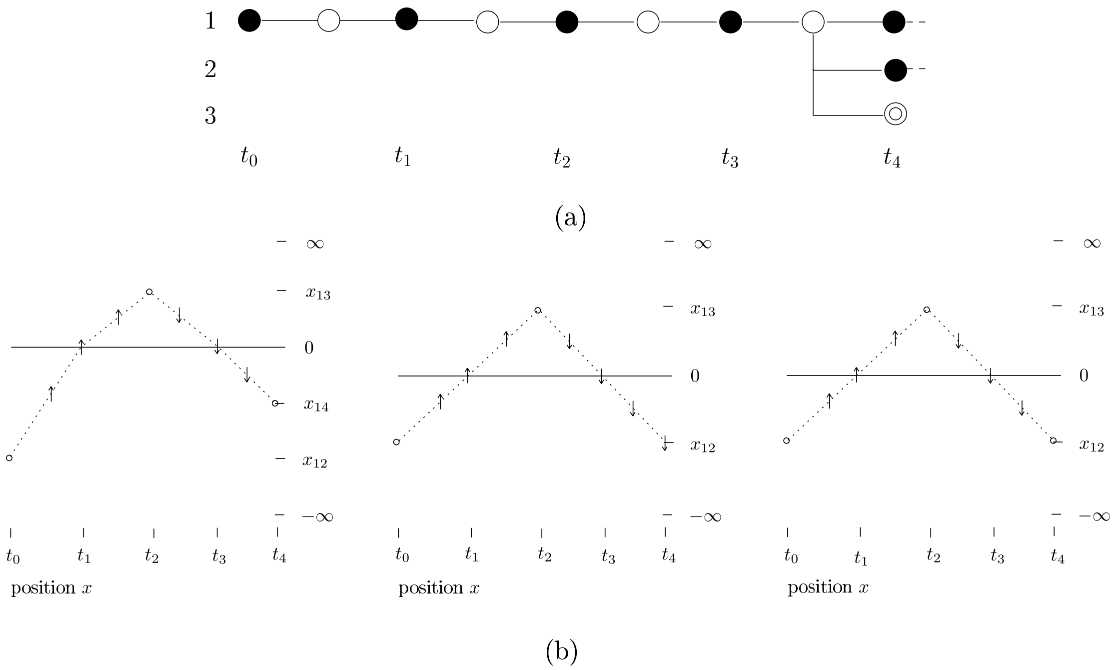


Figure 9 (a) Qualitative behavior tree for the undamped mass–spring system (see Figure 4 for the notation). (b) The temporal evolution of the position x of the spring in the three behaviors

builds upon earlier ideas on the use of higher-order time derivatives in qualitative simulation, such as de Kleer & Bobrow (1984) and Williams (1984c).

3.1.3 Spurious sequences of qualitative states

Spurious qualitative behaviors may also arise from the generation of an incorrect sequence of qualitative states by the QSIM algorithm. Contrary to the previous two cases, every individual state and state transition in the sequence is genuine. However, their succession yields a spurious behavior. Again, a simple example will serve to illustrate the point.

Consider an undamped mass–spring system with a linear spring force and unit mass, described by

$$\dot{x} = v, \tag{4}$$

$$\dot{v} = -kx. \tag{5}$$

As usual, the ODE model can be transformed into a QDE (not shown). Suppose we perform a qualitative simulation from an initial state in which the spring is compressed. Contrary to the previous examples, we now allow the introduction of new landmark values in the quantity spaces of the variables, replacing interval magnitudes at distinguished time-points. Figure 9 shows the behavior tree generated by QSIM for this model. The tree branches after t_3 to produce three possible qualitative behaviors at t_4. The first one represents a decreasing oscillation, the second one an increasing oscillation, and the third one a steady oscillation.

Although all three behaviors are consistent with the state and transition constraints, only the third behavior is a genuine possibility. One can easily show that the other two behaviors violate an implicit invariant: the sum of the potential and kinetic energy of the system. Since the total energy at t_4 must equal that at t_0, decreasing and increasing oscillations are impossible. The inclusion of the explicit energy function

$$E = \tfrac{1}{2}mv^2 + \tfrac{1}{2}kx^2$$

in the QDE of the mass–spring system, with E constant to reflect energy conservation, filters out the increasing and decreasing oscillations in Figure 9.

The energy conservation constraint is an example of a global constraint on the behavior of a system, a constraint which puts restrictions on the possible sequences of qualitative states up and above state constraints and transition constraints (Section 2.3.3). Global constraints can be made explicit and integrated into the qualitative simulation process to prune spurious qualitative behaviors from the behavior tree. Efforts in this direction have been guided to a large extent by insights and results from dynamic systems theory (Section 4). Examples of global constraints include energy constraints, or more generally Lyapunov functions (Fouché & Kuipers, 1992; Hofbaur &Dourdoumas, 2002), non-intersection constraints on trajectories in the phase space (Lee & Kuipers, 1988; Struss, 1988a), constraints on qualitative stability and instability (Ishida, 1989), constraints based on l'Hôpital's rule (Say, 1998), and analytical function constraints (Kuipers *et al.*, 1991).

3.2 *Combinatorial explosion of behavior trees*

As indicated in Section 2.4, qualitative simulation can give rise to ambiguous predictions of the behavior of the system. While some of the qualitative behaviors may be spurious, even the number of genuine qualitative behaviors can be too high to permit a useful interpretation of the simulation results. Two examples will illustrate how the qualitative nature of the models can lead to a multiplication of behavior predictions.

Consider the extended cascaded-tanks system in Figure 8(b). The system has two lower tanks filled from the same upper tank. It is described by the following differential equations:

$$\dot{a}_{\mathrm{u}} = i - f(a_{\mathrm{u}}, r_{\mathrm{u}}),\ f \in M^{++},$$
$$\dot{a}_{\mathrm{ll}} = f(a_{\mathrm{u}}, r_{\mathrm{u}}) - g(a_{\mathrm{ll}}, r_{\mathrm{ll}}),\ g \in M^{++},$$
$$\dot{a}_{\mathrm{lr}} = f(a_{\mathrm{u}}, r_{\mathrm{u}}) - h(a_{\mathrm{lr}}, r_{\mathrm{lr}}),\ h \in M^{++},$$

where the variables i, a, and r have the same meaning as before, and the suffixes $\cdot_{\mathrm{ll}}$ and $\cdot_{\mathrm{lr}}$ denote the lower-left and the lower-right tank, respectively. The incomplete specification of the functions g and h does not allow QSIM to unambiguously determine, when filling the tanks from empty, the order in which the water amounts in the lower tanks reach equilibrium. In fact, the qualitative direction of a_{ll} may become *std* before, after, or at the same time when the qualitative direction of a_{lr} becomes *std*. As a consequence, QSIM will generate qualitative behaviors for each of these cases, a phenomenon that has been called *occurrence branching* (Tokuda, 1996). In large and complex systems, with many processes occurring in parallel, occurrence branching can give rise to exponentially-growing behavior trees.

An obvious remedy to the combinatorial explosion of behavior trees due to occurrence branching is the abstraction of the QSIM output into higher-level descriptions of the qualitative behaviors of the system. One could argue that it does not really matter whether the lower-left or lower-right tank reaches equilibrium first, as the end result is the same: both tanks are at equilibrium. As a consequence, the alternative qualitative behaviors leading to the quiescent state might be collapsed into a description which abstracts from the order in which the tanks reach equilibrium. Several ways to ignore inessential qualitative distinctions have been proposed in the literature, such as the use of so-called *histories* for variables (Forbus, 1984; Williams, 1986; Coiera, 1992; Clancy & Kuipers, 1998) or the reduction of qualitative behavior trees by compacting several qualitative behaviors into a single abstract qualitative behavior (Weld, 1986; Mallory *et al.*, 1996; Tokuda, 1996; Eisenack & Petschel-Held, 2002).

Related ideas of abstraction underlie solutions to the problem of *chattering*, another cause of exponentially growing behavior trees. Chattering occurs when the qualitative value of a variable is totally unconstrained except by continuity, so that the QSIM algorithm is forced to repeatedly branch on every possible magnitude or direction (Kuipers & Chiu, 1987; Kuipers, 1994). An example of chattering occurs in a damped mass–spring system given by

$$\dot{x} = v, \tag{6}$$

$$\dot{v} = -kx - \mu v, \tag{7}$$

where μ denotes the friction constant ($\mu > 0$). When transforming the ODE model into a QDE, we introduce the auxiliary variable $a = \dot{v}$. By (7), $\dot{a} = -k\dot{x} - \mu\dot{v}$. Now, suppose that the system is in a qualitative state in which x is positive and *inc*, and v positive and *dec*. Whereas the magnitude of a is uniquely determined ($qmag_a =]-\infty, 0[$), its direction can be *dec*, *std*, or *inc*. Since there are no further constraints on the derivative of a, the transition constraints of Section 2.3.2 permit repeated transitions between qualitative states with $QV(a) = \langle]-\infty, 0[, dec \rangle$, $QV(a) = \langle]-\infty, 0[, std \rangle$, or $QV(a) = \langle$ for $]-\infty, 0[, inc \rangle$, thus exploding the behavior tree.[4] Clancy and Kuipers (1997b) have extended the basic QSIM algorithm with techniques for identifying chattering variables and abstracting a set of qualitative states involved in chattering into a single qualitative state with an unspecified qualitative direction.

3.3 Evaluation

Two major problems hampering the practical application of the QSIM method were discussed above: the occurrence of spurious qualitative behaviors and the combinatorial explosion of behavior trees. Much work in qualitative simulation has been directed at the improvement and extension of the QSIM algorithm to deal with these problems, as illustrated by the examples in the previous sections. This has resulted in a qualitative simulation method capable of dealing with a number of non-trivial systems, like physiological processes (Ironi *et al.*, 1990; Kuipers, 1989b; Ironi & Stefanelli, 1995; Rickel & Porter, 1997), (bio)chemical reactors (Molle & Edgar, 1990; Vinson & Ungar, 1995; Vatcheva, 2001) and chemical plants (Catino & Ungar, 1995), digital circuits (Kaul *et al.*, 1992), fatigue and fracture in steel bridges (Roddis & Martin, 1992), and genetic and ecological networks (Heidtke & Schulze-Kremer, 1998; Guerrin & Dumas, 2001a, b). Moreover, QSIM and its relatives have been embedded in broader reasoning tasks, such as monitoring and diagnosis (Forbus, 1987; Oyeleye *et al.*, 1990; DeCoste, 1991; Dvorak & Kuipers, 1991; Ng, 1991; Rose & Kramer, 1991; Lackinger & Nejdl, 1993; Vinson & Ungar, 1995; Dressler, 1996; Struss, 1997; Mosterman & Biswas, 1999; Panati & Dupré, 2000; Sachenbacher *et al.*, 2000), model composition (Falkenhainer & Forbus, 1991; Low & Iwasaki, 1992; Farquhar, 1994; Nayak, 1995; Levy *et al.*, 1997; Rickel & Porter, 1997), system identification (Söderman & Strömberg, 1991; Varšek, 1991; Richards *et al.*, 1992; Hau & Coiera, 1993; Shen & Leitch, 1995; Bradley & Stolle, 1996; Say & Kuru, 1996; Capelo *et al.*, 1998; Bellazzi *et al.*, 1999; Šuc *et al.*, 2003; Šuc & Bratko, 2003; Coghill *et al.*, 2004), theory refinement and measurement analysis (Kamps & Péli, 1995; de Jong *et al.*, 1999), tutoring (Forbus, 1997; de Koning *et al.*, 2000; Bredeweg & Forbus, 2003; Salles *et al.*, 2003), and comparative analysis (Weld, 1988, 1990a, b, 1992; Neitzke & Neumann, 1994; de Jong & van Raalte, 1999; Struss, 2004).

The improvements and extensions of the basic QSIM algorithm can eliminate some spurious qualitative behaviors. However, Say recently demonstrated that the development of a qualitative simulator that is both sound and complete, in the sense of Section 2.5, is impossible (Say & Akin, 2003). In fact, an algorithm for generating all and only genuine qualitative behaviors, given a qualitative model and initial qualitative state, could be used to solve Hilbert's tenth problem, that is, decide whether a given multivariate polynomial with integer coefficients has integer solutions. As

[4] As an aside, it is remarked that the higher-order derivative constraint discussed in Section 3.1.2 is to no avail in this case. The cause of chattering does not lie in the failure to exploit information implicit in the model, but rather in the absence of this information.

it has been proven that an algorithm for solving Hilbert's tenth problem does not exist, the generation of spurious qualitative behaviors cannot be excluded.

While QSIM is thus inherently incomplete, for practical purposes it would already be satisfactory to have a qualitative simulator that filters out as many known classes of spurious behaviors as possible. In order to achieve this, mathematical constraints on the possible qualitative behaviors of the system have to be expressed as qualitative constraints or integrated in the simulation algorithm. Unfortunately, the efforts to improve QSIM are complicated by fundamental design decisions underlying the method (Sacks, 1990b; Makarovic, 1991; Sacks & Doyle, 1992). For example, the abstraction of an ODE model into sets of qualitative constraints may facilitate the efficient computation of qualitative states, but makes it difficult to apply mathematical techniques based on algebraic manipulation of the model equations. The examples in this section illustrate that such algebraic reasoning is critical for filtering out spurious qualitative behaviors, through the decomposition of an ODE into different sets of basic equations (Section 3.1.1), the derivation of expressions for higher-order time derivatives (Section 3.1.2), or the formulation of equations that express energy conservation laws (Section 3.1.3).

Even if all spurious qualitative behaviors could be ruled out, the behavior tree resulting from a simulation may still be intractable. In the absence of sufficiently-tight mathematical constraints, the number of qualitative behaviors is expected to explode, especially when dealing with large and complex systems. The techniques mentioned in Section 3.2 may alleviate the problem to some extent, but cannot avoid that the upscalability of qualitative simulation to interesting problems in the real world will be difficult to achieve. In order to reduce the number of possible qualitative behaviors of the system, further information is required, for example order-of-magnitude or numerical constraints. Being purely qualitative, the QSIM algorithm described in the previous section is not able to exploit any such available information.

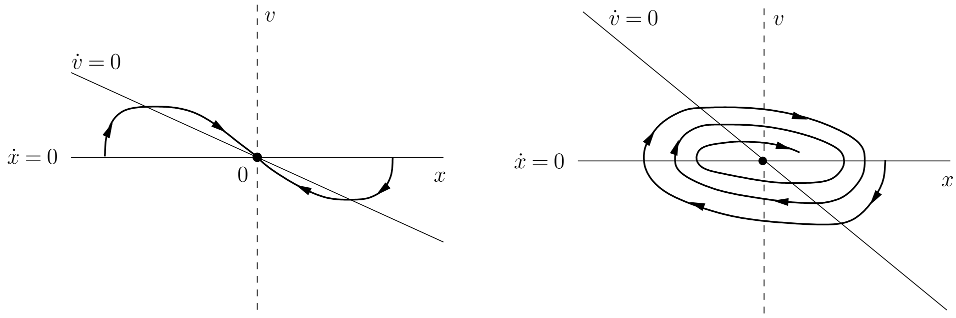
We conclude that the occurrence of spurious qualitative behaviors and the combinatorial explosion of behavior trees are problems difficult to resolve in the framework of QSIM and other qualitative simulation methods. In the next section, we will discuss two related approaches that address these problems by changing the perspective on qualitative simulation. The first approach redefines qualitative simulation in the framework of dynamic systems theory, in order to optimally exploit mathematical techniques available for certain classes of dynamic systems. Some of the methods focus on quantitative instead of qualitative models. The second approach also goes beyond the purely qualitative framework, by generalizing qualitative simulation to semi-quantitative simulation. The two approaches have been shown capable of making useful predictions about the behavior of large and complex systems.

4 Qualitative phase-space analysis

4.1 Overview

Dynamic systems theory is a branch of mathematics that has developed powerful techniques for the qualitative analysis of dynamic systems (Hirsch & Smale, 1974; Guckenheimer & Holmes, 1987; Strogatz, 1994). These techniques help provide a high-level view of the qualitative dynamics of a system by identifying equilibrium points, limit cycles, and other attractors in the phase space, as well as by determining their stability and basin of attraction. In addition, the techniques allow the study of changes in parameter values, particularly those leading to bifurcations involving changes in the number or character of the attractors. Probably the best-known result of dynamic systems theory is the characterization of the phase-space behavior of second-order linear systems in terms of the sign of the eigenvalues of the state matrix. This result is generalizable to higher-order linear systems, while other techniques apply to particular classes of nonlinear systems.

Consider again the damped mass–spring system (6)–(7). We can rewrite the equations in the form



(a) (b)

Figure 10 Example solution trajectories of the damped mass–spring system, for (a) $\mu^2>4k$ *and (b)* $\mu^2<4k$

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} x \\ v \end{bmatrix} = A\begin{bmatrix} x \\ v \end{bmatrix}, \quad \text{with } A = \begin{bmatrix} 0 & 1 \\ -k & -\mu \end{bmatrix}. \tag{8}$$

This linear system has a single equilibrium point, (0, 0). The stability of the equilibrium can be determined from inspection of the eigenvalues of A:

$$\lambda = \frac{-\mu \pm \sqrt{\mu^2 - 4k}}{2}.$$

In fact, since the real part of the eigenvalues is negative, the equilibrium point is stable. Moreover, if $\mu^2>4k$, then the eigenvalues are real, and an initial displacement is followed by an overdamped return to the equilibrium. On the other hand, if $\mu^2<4k$, then the eigenvalues have a real and an imaginary part, and the system oscillates back towards the equilibrium in an asymptotic manner.[5] Figure 10 shows example solutions for the above two cases as trajectories in the (x, v)-phase plane. The nullclines $\dot{x}=0$ and $\dot{v}=0$ divide the phase plane into four regions, in each of which the dynamics of a system is characterized by a unique sign for $\dot{x}$ and $\dot{v}$.

The example demonstrates how simple mathematical techniques permit the qualitative behavior of the mass–spring system to be analyzed in an elegant and precise way (see Stoker (1992) for techniques applying to nonlinear variants of this system). In contrast, treatment of the same system by QSIM is less straightforward. It requires energy constraints (Fouché & Kuipers, 1992; Kuipers, 1994) that are cumbersome to express in the QDE formalism, as well as mechanisms to detect and eliminate chattering variables (Section 3). Moreover, the resulting behavior tree does not adequately describe the asymptotic behavior of the system, in the sense that it includes spurious behaviors in which the equilibrium point is not reached asymptotically, but in finite time, after a finite number of oscillations. While these behaviors may occur for some nonlinear mass–spring systems, they do not correspond to any solutions of the linear system (8).

Reformulations of the QSIM approach in the framework of dynamic systems theory (Aubin, 1989; Sacks, 1990b; Dordan, 1992; Lee & Kuipers, 1993) show that the conclusions we arrived at in the simple example above apply more generally. In many situations, the QSIM predictions of the qualitative behaviors of a dynamic system are weaker than those obtained by techniques developed in dynamic systems theory. Besides being a touchstone for the critical evaluation of work on qualitative simulation, the perspective of dynamic systems theory has also provided a basis for the development of alternative methods (Abelson *et al.*, 1989; Sacks, 1990b; Kalagnanam *et al.*, 1991). Several such *qualitative phase-space analysis* methods have been proposed since the early 1990s. Contrary to QSIM and its relatives, these methods are tailored to a particular class of dynamic

[5] For $\mu^2=4k$ the system is critically damped and the solutions resemble those for the overdamped case.

systems, in order to optimally exploit any strong mathematical constraints available for these systems. This reduces the occurrence of spurious and uninformative behavior predictions.

The first type of qualitative phase-space analysis method deals with numerical instead of qualitative models. Given an ODE, numerical parameter values, and a numerical bounding box for the state, these methods derive the phase-space behavior of the system using a combination of symbolic and numerical techniques. While the models being treated are numerical, it is nevertheless appropriate to label the methods as qualitative. Although numerical techniques lie at the heart of the approaches, their fundamental aim is to obtain qualitative insight into the dynamics of the system. The results of the methods do not simply consist of a set of solution trajectories. Instead, the methods provide an account of the possible qualitative behaviors of the system, phrased in terms of concepts like equilibrium point, limit cycle, stability, and bifurcation. In comparison with well-known mathematical problem solvers such as Maple, Mathematica, and Matlab, the phase-space analysis programs add a layer of knowledge representation and task control allowing the coordinated application of a range of low-level numerical routines. A disadvantage of the methods is that a soundness guarantee like that in QSIM cannot be given.

Two examples of implemented numerical phase-space analysis methods are KAM (Yip, 1991a, b) and MAPS (Zhao, 1993, 1994). The KAM program is concerned with the automatic qualitative analysis of nonlinear Hamiltonian systems with two degrees of freedom. In one instance, the use of KAM has led to previously unknown results in hydrodynamics. MAPS is a program constructing a qualitative description of the phase-space structure of nonlinear systems. Although the computational complexity of the method has limited its application to second-order and third-order systems, the underlying concepts and algorithms apply to higher-order systems as well. Together with Perfect Moment, which analyzes a system's phase-space behavior with special attention to chaotic features (Bradley, 1995), MAPS has been used for nonlinear control design (Bradley & Zhao, 1993). Other examples of numerical phase-space analysis methods are POINCARE (Sacks, 1991; see Abelson (1990) for a precursor), and PSX2NL (Nishida, 1997; see Nishida (1993, 1994) and Nishida & Doshita (1995) for results obtained with relatives and extensions of PSX2NL).

The models treated by the second type of qualitative phase-space analysis method are qualitative in nature, comparable to the QSIM models. An example is the qualitative phase-space analysis method of Bernard and Gouzé (1995, 2002), which will be discussed in more detail in Section 4.2. It derives the qualitative transient and asymptotic behavior of loop-structured systems with monotonic interactions, a class of systems occurring in numerous applications in biology. A bit older, but still of considerable interest is the PLR program of Sacks (1990a). PLR automates the qualitative analysis of second-order systems using piecewise-linear approximations of nonlinear functions. It uses an inequality reasoner allowing the flexible integration of numerical information (Sacks, 1987). Another example is the method of Dordan (1992, 1995), which is a reformulation of QSIM for so-called replicator systems, used in chemistry and ecology. de Jong and colleagues (de Jong & Page, 2000; de Jong *et al.*, 2002, 2004b) have developed a method for the qualitative simulation of genetic regulatory networks described by a class of piecewise-linear differential equations. The method has been implemented in the computer tool GNA and applied to complex networks of biological interest (de Jong *et al.*, 2003, 2004a). Because there usually exist strong mathematical constraints on the possible qualitative behaviors, the methods are able to deal with quite complex second-order, and sometimes higher-order, systems.[6] For example, the program GNA has been used to simulate genetic regulatory networks with a dozen state variables. Generally speaking though, upscaling is limited by the qualitative nature of the models.

[6] Although not directly based on dynamic systems theory, the methods in Capelo *et al.* (1998) and Schaefer (1991) are similar in spirit, in that they attempt to exploit the properties of a particular class of systems.

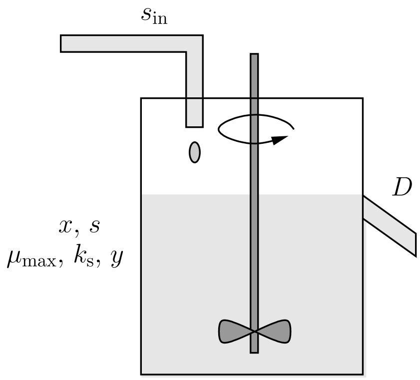


Figure 11 Schematic view of a chemostat. The variables denote the total amount x of biomass per unit volume and the concentration s of remaining nutrient. The parameters are the dilution rate D, the input nutrient concentration s_{in}, the maximum growth rate $\mu_{\max}$ of cells, a half-saturation constant k_{s}, and the growth yield y

4.2 Qualitative analysis of loop-structured systems

Bernard & Gouzé (1995, 2002) have developed a method for the qualitative analysis of *loop-structured systems* with monotonic interactions. Examples of loop-structured systems, frequently occurring in biology, are the feedback mechanisms regulating protein synthesis and the development of stage-structured populations. More precisely, loop-structured systems are defined by ODEs of the form $\dot{\boldsymbol{x}}=\boldsymbol{f}(\boldsymbol{x})$, with $\boldsymbol{x}=[x_1, \ldots, x_n]'$ and $\boldsymbol{f}=[f_1, \ldots, f_n]'$, while f_i:$\Omega\rightarrow\mathbb{R}$ is a continuously differentiable function, with Ω an open convex domain of $\mathbb{R}^n$, and

$$f_i(\boldsymbol{x})=f_i(x_i,\ x_{i+1}),\ 1\leq i\leq n,$$

where the indices are numbered modulo n. That is, the variables are ordered in a loop, such that the derivative of each variable is determined by the variable itself and its successor. The Jacobian matrix M of loop-structured systems has the following structure:

$$M(x) = \begin{bmatrix} m_{11}(x) & m_{12}(x) & 0 & \cdots & 0 & 0 \\ 0 & m_{22}(x) & m_{23}(x) & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & m_{n-1,n-1}(x) & m_{n-1,n}(x) \\ m_{n,1}(x) & 0 & 0 & \cdots & 0 & m_{n,n}(x) \end{bmatrix}, \tag{9}$$

where $m_{ij}(\boldsymbol{x})=(\partial/\partial x_j)f_i(\boldsymbol{x})$. Note that every two-dimensional system is by definition loop-structured. A loop-structured system is said to have *monotonic interactions* on Ω, if m_{ij}, $i\neq j$, does not change sign on Ω (similar to the monotonic functions used in QSIM). The discussion below is restricted to loop-structured systems with monotonic interactions. However, slight deviations from this structure may still allow the method to yield useful predictions of the qualitative behavior of the system.

An example of a loop structured system is the growth of microorganisms in a chemostat. The chemostat is a type of bioreactor in which nutrient supply and other conditions can be controlled (Figure 11). This system can be described on $\Omega=\mathbb{R}^2_+$ by the so-called *Monod model*:

$$\dot{x}=\mu(s)x - Dx, \tag{10}$$

$$\dot{s}=D(s_{\mathrm{in}}-s)-\rho(s)x, \tag{11}$$

where x denotes the total amount of biomass per unit volume and s the concentration of remaining nutrient. D and s_{in} are parameters representing the dilution rate and the input nutrient concentration, respectively ($D>0$, $s_{\text{in}}>0$). The functions $\mu(s)$ and $\rho(s)$ are defined as follows:

$$\mu(s) = \mu_{\max} \frac{s}{s + k_{\text{s}}} \quad \text{and} \quad \rho(s) = \frac{1}{y}\mu(s),$$

with $\mu_{\max}$ the maximum growth rate of cells, k_{s} a half-saturation constant, and y the growth yield ($\mu_{\max}>0$, $k_{\text{s}}>0$, $y>0$). The system described by the Monod model has monotonic interactions, since the off-diagonal elements of its Jacobian matrix have a fixed sign in Ω (($x\ \mu_{\max}\ k_s/(s+k_s)^2>0$ and $-\rho(s)<0$).

Let $\boldsymbol{x}^*\in\Omega$ be an equilibrium point of the system. This equilibrium point lies on the intersection of hyperplanes defined by

$$V_i(\boldsymbol{x}^*)=\{\boldsymbol{x}\in\Omega | x_i=x_i^*\}.$$

The hyperplanes associated with $\boldsymbol{x}^*$ divide the phase space into 2^n so-called *$\boldsymbol{x}^*$-orthants* W_k ($\boldsymbol{x}^*$), $1\leq k\leq 2^n$.[7] In each $\boldsymbol{x}^*$-orthant, the sign of the difference $x_i - x_i^*$ is constant. The system is called *diagonally $\boldsymbol{x}^*$-monotonic*, if the sign of the diagonal elements of the Jacobian matrix M is constant in every $\boldsymbol{x}^*$-orthant of the phase space. Figure 12 shows the $\boldsymbol{x}^*$-orthants of the Monod model (10)–(11) with respect to its (single) equilibrium point in Ω, denoted by (x^*, s^*) (Bernard, 1995). As can be easily verified, the Monod system is diagonally monotonic with respect to this equilibrium.

In a similar way, the phase space can be divided into so-called z -orthants Z_l, $1\leq l\leq 2^n$, by means of the *nullclines*:

$$U_i=\{\boldsymbol{x}\in\Omega | f_i(\boldsymbol{x})=0\}.$$

A region in Ω that is an intersection of an $\boldsymbol{x}^*$-orthant and a z-orthant can be interpreted as the phase-space analog of a qualitative state in the QSIM formalism. In this region, the relative position vector and the velocity vector have a unique sign.

The computation of the possible qualitative states of a diagonally monotonic loop-structured system amounts to determining, for each $\boldsymbol{x}^*$-orthant $W_k(\boldsymbol{x}^*)$, the z-orthants Z_l that it intersects with. This is achieved by the theorems in Bernard & Gouzé (2002), which allow the qualitative states to be computed from the signs of the elements of the Jacobian matrix M (Figure 12(c)). The possible transitions between the qualitative states are also determined from the sign properties of M, by formulating criteria for the crossing of a hyperplane $V_i(\boldsymbol{x}^*)$ (i.e. x_i reaches its equilibrium value from above or below) or for the crossing of a nullcline U_i (i.e. x_i reaches a minimum or a maximum) (Bernard & Gouzé, 2002). Transitions characterized by the simultaneous occurrence of two qualitative events, for example the simultaneous crossings of two hyperplanes $V_i(\boldsymbol{x}^*)$ and $V_j(\boldsymbol{x}^*)$, $i\neq j$, are generally excluded, except in special cases when the set of trajectories corresponding to these transitions are not of measure 0. Additional constraints on transitions are obtained from theorems on the global qualitative behavior of loop-structured systems. The qualitative states and transitions between qualitative states can be visualized in the form of a *transition graph* (also called *envisionment* in qualitative simulation; Forbus, 1984; Kuipers, 1994). Each state is represented by an $n\times 2$-matrix of signs. The first column lists the position of every x_i with respect to its equilibrium value x_i^* (+meaning $x_i>x_i^*$, while − meaning $x_i<x_i^*$). The second column lists the sign of every $\dot{x}_i$. The transitions between the states are denoted by arrows.

The transition graph for the Monod model is shown in Figure 13(a). The graph contains a cycle, which might lead one to believe that there exist limit cycles or trajectories spiraling to or from an

[7] The analysis can be easily generalized to the case of multiple equilibrium points, by introducing separate hyperplanes for each equilibrium point.

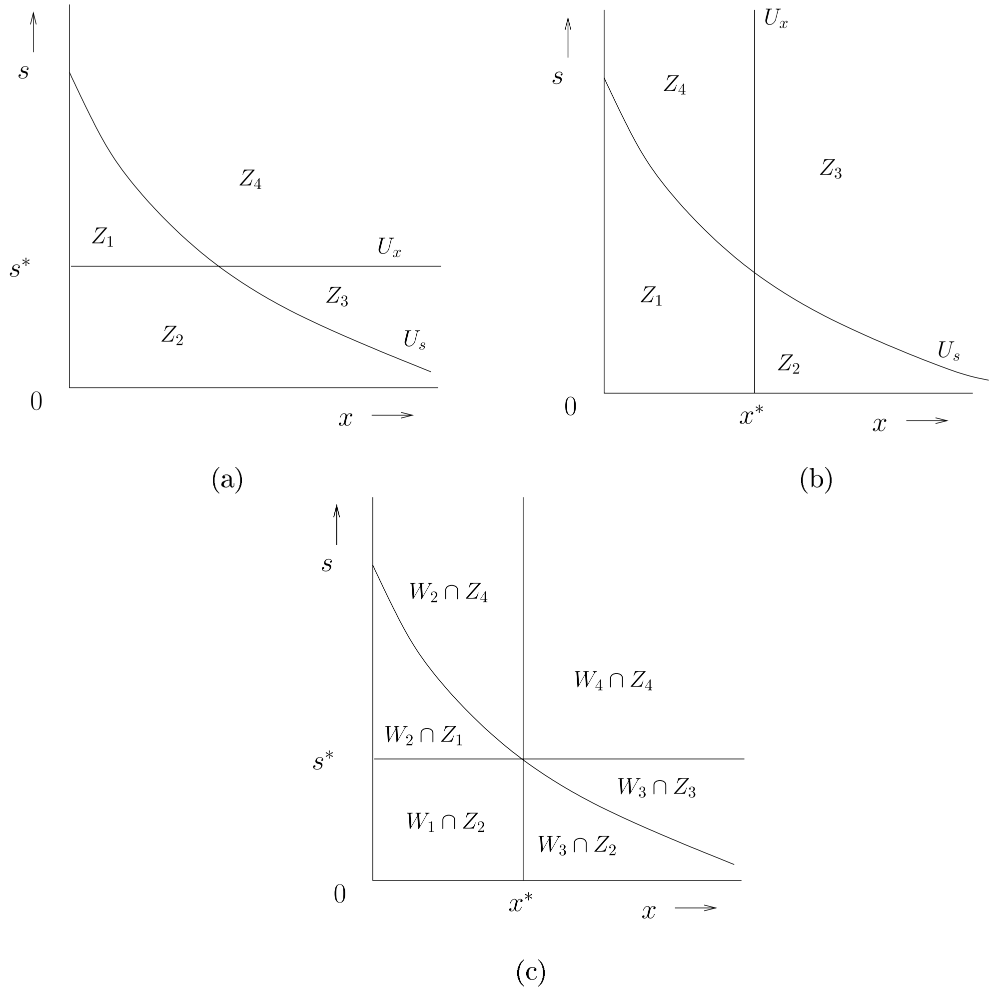


Figure 12 Subdivision of the phase space of the chemostat system in Figure 11, described by the Monod model, into (a) $\boldsymbol{x}$*-orthants, (b) z-orthants, and (c) intersections of $\boldsymbol{x}$*-and z-orthants. V_s $(x^*, s^*)=\{(x, s) \in \Omega | s=s^*\}$, V_x $(x^*, s^*)=\{(x, s) \in \Omega | x=x^*\}$,$U_s=\{(x, s) \in \Omega | \dot{s}=0\}$, and $U_x=\{(x, s) \in \Omega | \dot{x}=0\}$. Furthermore, $Z_1=\{(x, s) \in \Omega | \dot{x}>0, \dot{s}>0\}$, $Z_2=\{(x, s) \in \Omega | \dot{x}<0, \dot{s}>0\}$, $z_3=\{(x, s) \in \Omega | \dot{x}<0, \dot{s}<0\}$, and $Z_4=\{(x, s) \in \Omega | \dot{x}>$o, $\dot{s}<0\}$

equilibrium point in Ω. However, further analysis reveals that the cycle is spurious, due to ignoring an implicit constraint in the model. In fact, the graph can be refined by taking into account the additional variable $u=s+(x/y)$, denoting the total nutrient concentration in the chemostat. From (10) and (11) it follows that

$$\dot{u}=D(s_{\mathrm{in}}-u). \tag{12}$$

Depending on whether the initial value u_0 of u is above or below s_{in}, $\dot{u}$ is negative or positive. The sign of $\dot{u}$ puts additional restrictions on the possible behaviors allowed by the Monod model (Bernard, 1995). For instance, if $\dot{u}$ is positive, the states in which x and s simultaneously decrease can be excluded. Upon considering the two cases $\dot{u}>0$ and $\dot{u}<0$ separately, the original transition graph refines to the two transition graphs shown in Figure 13(b). In both cases, the system converges towards the equilibrium. However, in the former case, x passes through a minimum and s through a maximum, whereas in the latter case, x passes through a maximum and s through a minimum.

Like QSIM, the phase-space analysis method of Bernard and Gouzé determines possible qualitative states and transitions between qualitative states. However, the definition of qualitative

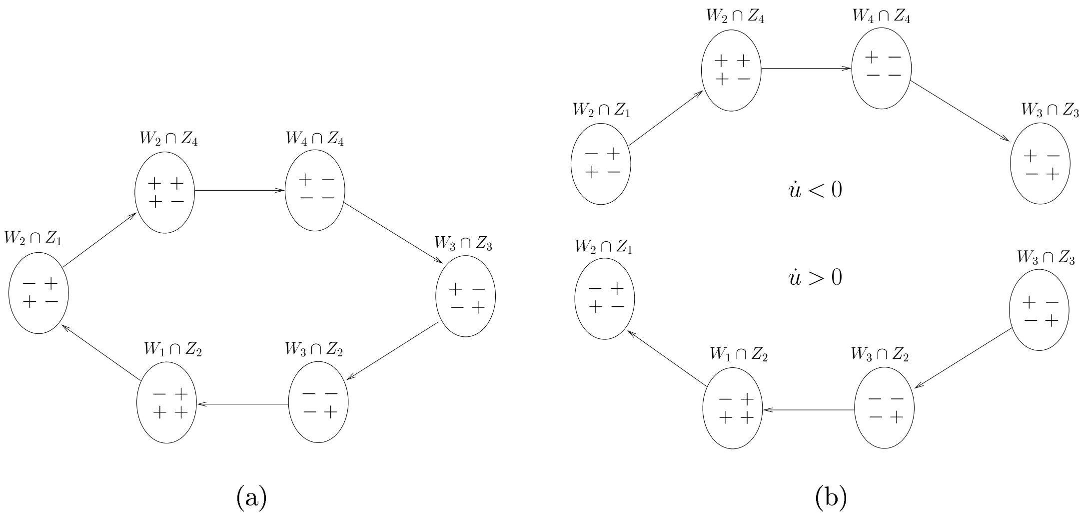


Figure 13 Transition graphs derived for the Monod model (Bernard, 1995). In (a) the variable u for the total nutrient concentration is not taken into account, whereas in (b) it is, leading to two refined transition graphs. The first column in the sign matrix characterizing a state gives the position of the variables with respect to their equilibrium value, whereas the second column gives the sign of the derivative of the variables. The first row of the matrix concerns the variable x and the second row the variable s

state is based on a more appropriate, not necessarily hyperrectangular decomposition of the phase space. In addition, the computation of qualitative states and transitions between qualitative states has been tailored to the loop-structured systems under study. This reduces the risk of generating uninformative or spurious states and transitions between states. Theorems similar to the soundness property of QSIM (Section 2.5) have been derived for the qualitative analysis of loop-structured systems (Bernard & Gouzé, 1995). The chemostat example concerns a two-dimensional system, but the method applies to loop-structured systems of dimension n.

The method discussed in this section has been used for the analysis of a range of biological systems for which no or only weak quantitative information is available (Bernard & Gouzé, 1995, 1996, 1999; Bernard & Souissi, 1998). For example, it has been applied in the validation of a third-order model of the response of a population of phytoplankton to a periodic input of nutrient (Bernard & Gouzé, 1999). By comparing the predicted sequences of qualitative states with observed qualitative trends, it was found that the phytoplankton growth models are appropriate for low-frequency input, but break down at high frequency.

5 Semi-quantitative simulation

5.1 Overview

ODEs and QDEs are the two extremes of a scale running from complete to no numerical information. Most situations of practical interest, however, fall somewhere in between these two extremes. In fact, for many scientific and engineering problems, some numerical information on parameter values and functional relationships is available. This additional information can be exploited to arrive at better predictions than those obtainable through qualitative simulation alone.

A first example of such information is the *order of magnitude* of the value of parameters and variables in the model. Basically, two kinds of order-of-magnitude information can be distinguished: absolute and relative (Travé-Massuyès & Dague, 2003; Travé-Massuyès *et al.*, 2003). Whereas *absolute* orders of magnitude relate the value of a parameter or variable to a set of real-measured landmarks, e.g. by labeling it as 'large negative', 'small negative', 0, 'small positive', or 'large positive' *relative* orders of magnitude compare the values of two parameters or variables, e.g. by stating that one is 'negligible with respect to', 'close to', or 'comparable to' the other

(Mavrovouniotis & Stephanopoulos, 1988; Travé-Massuyès & Piera, 1989; Raiman, 1991; Dague, 1993a, b). Order-of-magnitude relations can be formalized by means of axioms that, when supplemented with appropriate inference rules, allow some of the ambiguities arising from the use of qualitative methods to be resolved.

Consider, for instance, the damped mass–spring system of Section 4.1. If we just know that $k>0$ and $\mu>0$, we cannot distinguish between the two qualitative behaviors summarized in Figure 10. However, suppose that we know that $4k$ is a 'small positive' and μ^2 is a 'large positive'. Then one of the behavorial possibilities, the oscillation of the mass around the equilibrium position, can be excluded. A similar conclusion can be drawn when $4k$ is 'negligible with respect to' μ^2. Order-of-magnitude reasoning has been given a solid mathematical foundation by defining the relations between parameters and variables in the framework of standard or non-standard real analysis (see Robinson (1966) for an introduction to non-standard analysis). However, its application to qualitative simulation seems to have been limited (see Davis (1990) for an exception).

More widely used is the second kind of numerical information, which specifies real intervals for the values of parameters and variables, and in some cases, real envelopes for functional relationships. Suppose that in the mass–spring example numerical bounds on the value of k and μ were available, e.g. $k\in[0.001, 0.002]$ and $\mu\in[0.1, 0.3]$. Using interval arithmetic (Moore, 1979), a generalization of conventional real arithmetic, it follows that $4k\in[0.004, 0.008]$ and $\mu^2\in[0.01, 0.09]$, and hence $4k<\mu^2$, which again excludes the oscillatory behavior. The use of intervals allows numerical uncertainty to be represented in a flexible way. Since the interval formalism includes exact values (e.g. $k\in[0.001, 0.001]$) and sign values (e.g. $k\in\,]0, \infty[$) as special cases, it constitutes a unifying framework for the representation of both qualitative and quantitative information. Several methods for *semi-quantitative* (or *semi-qualitative*) *simulation* have been proposed in the literature, which can be roughly divided into two approaches.

The first approach, which will be called *qualitative–quantitative* simulation, uses numerical information to refine the behavior tree obtained through qualitative simulation. More precisely, the methods compute interval bounds for the landmark values of the system variables. This may lead to the refutation of qualitative behaviors inconsistent with the numerical information, and hence to a reduced behavior tree. In addition, the numerical information can be used to estimate the probability of alternative transitions from a state, and hence prioritize qualitative behaviors (Doyle & Sacks, 1991; Grossman & Werther, 1993; Leitch & Shen, 1993). The most well-known qualitative-quantitative methods are Q2, Q3, and NSIM. Q2 (Berleant & Kuipers, 1992; Kuipers, 1994) acts as a filter on the qualitative states in a behavior, generating interval constraints from the QSIM model and propagating interval bounds through the constraints. Q3 (Berleant & Kuipers, 1997) improves upon Q2 by adding interval constraints obtained from a refinement of the time step between consecutive distinguished time-points. Q2 and Q3 will be discussed in Section 5.2. Q2 and Q3 can be used in combination with NSIM (Kay & Kuipers, 1993), which computes numerical envelopes for the solutions of a semi-quantitative model. Q2 and NSIM have been integrated into the simulator SQSIM (Kay, 1998). The above extensions of QSIM have been applied in the context of model-based reasoning tasks like monitoring (Dvorak & Kuipers, 1991; Rinner & Kuipers, 1999), system identification (Kay *et al.*, 2000), comparative analysis (Vatcheva & de Jong, 1999), and experiment selection (Vatcheva *et al.*, 2000, 2001).

A second approach towards semi-quantitative simulation does not take the qualitative behaviors produced by QSIM or another qualitative simulator as its starting point. Given an ODE model with interval bounds on the parameters and initial conditions, the methods compute interval bounds on the state variables at successive time steps. Starting with the pioneering work of Moore (1979), a variety of such *interval simulation* methods have been proposed (e.g. Vescovi *et al.*, 1995; Lohner, 1987; Nedialkov & Jackson, 1999a; Janssen *et al.*, 2001; for recent reviews, see Nedialkov & Jackson, 1999b; Armengol *et al.*, 2000; Jackson & Nedialkov, 2002).[8] The methods provide more

[8] Similar methods for semi-quantitative simulation have been developed in the context of fuzzy simulation (Bousson & Travé-Massuyès, 1993; Shen & Leitch, 1993; Bonarini & Bontempi, 1994). This has, for example,

or less satisfactory solutions for the major problem of semi-quantitative simulation: the tendency of interval bounds to explode as the number of time steps increases, especially for large interval bounds of the parameters and initial conditions. One way to deal with this problem is represented by Lohner's AWA system (Lohner, 1987), which employs coordinate transformations to counter the *wrapping effect*, the loss of precision entailed by the approximation of an arbitrary region by a bounding box. Recently, Janssen *et al.* (2001, 2002) have proposed sophisticated constraint satisfaction algorithms to reduce the size of bounding boxes at successive time-points. Examples of real-world applications of the interval simulation methods mentioned in this paragraph are the monitoring of a sintering process in a steel plant (Vescovi *et al.*, 1997) and a gas turbine in a chemical plant (Travé-Massuyès & Milne, 1997).

In comparison with QSIM and its numerical extensions, interval simulation produces quantitative predictions without imposing an overarching qualitative framework. In particular, it does not describe the behavior of the system in terms of sequences of distinguished time-points, where variables attain landmarks or extrema. This has the disadvantage that qualitatively different behaviors are not recognized, which may give rise to broad interval bounds covering several such behaviors. Moreover, the absence of a qualitative representation makes it more difficult to discern meaningful patterns in the large amounts of numerical data.

One could imagine enhancing interval simulation by the parallel execution of a qualitative and a (semi-)quantitative simulation. Several methods realizing this latter idea have been proposed in the literature, such as the *self-explanatory simulation* method of Forbus and Falkenhainer (Forbus & Falkenhainer, 1990, 1992, 1995; Amador *et al.*, 1993; Iwasaki & Low, 1993). The aim of self-explanatory simulation is to provide better explanations of the system behavior, ensure consistency of the predictions with the underlying domain knowledge, and automate the model-building process (see Forbus (1997) for an application in the field of tutoring). Related ideas, but generalized to spatio-temporal dimensions, have informed methods for the analysis of spatio-temporal data sets developed by Yip, Zhao, and colleagues (Yip, 1995, 1997; Yip & Zhao, 1996; Ordóñez & Zhao, 2000; Bailey-Kellogg & Zhao, 2001, 2003) (see Junker & Braunschweig (1995) for related work). For example, the spatio-temporal aggregation (STA) system recognizes and tracks qualitative structures in data sets, resulting from the simulation of reaction-diffusion systems in two spatial dimensions (Ordóñez & Zhao, 2000). STA additionally samples the parameter space and generates equivalence classes of qualitatively similar behaviors. It thus rejoins the qualitative phase-space analysis methods mentioned in Section 4.1, generalizing their scope to spatial in addition to temporal dimensions.

5.2 Semi-quantitative simulation with Q2 and Q3

Among the best known semi-quantitative simulation methods are *Q2* and *Q3*, developed by Berleant and Kuipers (Berleant & Kuipers, 1992, 1997; Kuipers, 1994). Q2 and Q3 assume that the system being considered is described with a *semi-quantitative differential equation (SQDE)* model. An SQDE is a QDE augmented by numerical information, in particular interval bounds for landmark values l and bounding envelopes for functional relations f. An interval bound for l is given by *range* $(l)=[\underline{l}, \bar{l}]$, where $\underline{l}, \bar{l} \in \mathbb{R}^*$ and $\underline{l} \leq l \leq \bar{l}$. A bounding envelope for f is defined by *envelope*$(f)=[\underline{f}, \bar{f}]$, such that for all x in the domain of the function, it holds that $\underline{f}(x) \leq f(x) \leq \bar{f}(x)$. Furthermore, interval bounds on the first- and second-order derivative of f may be specified.

In Figure 14 the SQDE for a nonlinear variant of the mass–spring system in Figure 5 is shown. The SQDE corresponds to the differential equations

$$\dot{x} = v,$$

$$\dot{v} = -kf(x), \ f \in M_0^+,$$

resulted in a simulation method capable of treating time-delayed semi-quantitative differential equations (Miguel & Shen, 2005).

(a)	(b)
$\mathrm{D/DT}(v, x)$	
$\mathrm{D/DT}(a, v)$	
$\mathrm{MULT}(-k, fx, a)$	
$\mathrm{MINUS}(k, -k)$	
$\mathrm{M}_0^+(x, fx)$	$envelope(f) = [x + x^3/6 - 1, x + x^3/6 + 1]$
$\mathrm{CONSTANT}(-k)$	
$\mathrm{CONSTANT}(k)$	$range(k) = [0.08, 0.13]$

Figure 14 (a) QDE abstracted from the nonlinear ODE model of the mass–spring system in Figure 5 (the quantity spaces of the variables have been omitted). (b) Interval bounds of the parameter k and bounding envelope of the function f

which have been abstracted into qualitative constraints, as explained in Section 2.2. The resulting QDE has been augmented with interval bounds for k and envelope functions for f.

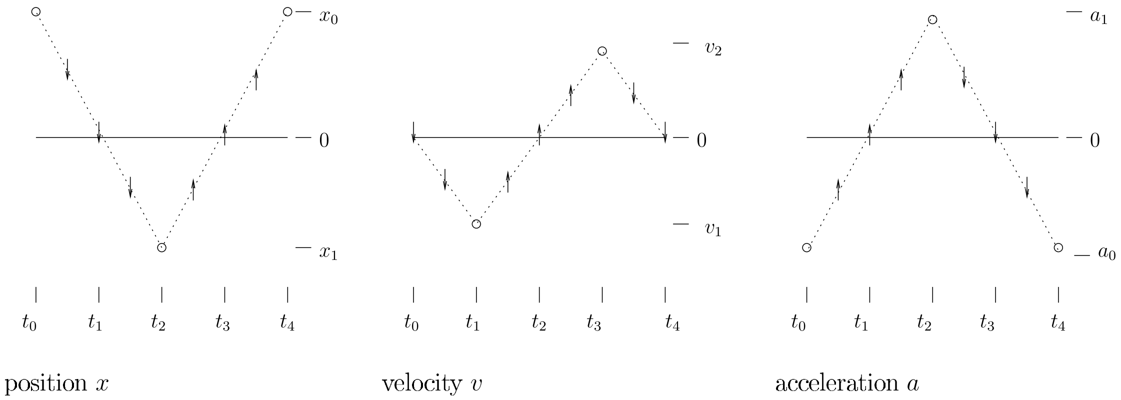
Q2 refines the qualitative behavior tree produced by QSIM by propagating the numerical information contained in the SQDE. Given a qualitative behavior $QS(t_o)$, $QS(t_o)$, t_l, $QS(t_l)$, . . ., $QS(t_p)$, Q2 first derives equations and inequalities, involving the landmarks of the system variables, from the qualitative values in $QS(t_i)$, $1 \le i \le p$, and from the qualitative constraints in the QSIM model. For example, if at t_i the variable x has the landmark value l, then the equation $x(t_i)=l$ is generated. The qualitative constraint MULT(x, y, z) leads to the equation $x(t_i)\, y(t_i)=z(t_i)$, while the monotonic function constraint $\mathrm{M}^+(x, y)$, for which the envelope functions $\underline{f}$ and $\bar{f}$ have been defined, gives rise to the inequalities $\underline{f}(x(t_i)) \le f(x(t_i)) \le \bar{f}(x(t_i))$. Also, for the derivative constraint D/DT (x, y) the equality

$$x(t^*) = \frac{y(t_i) - y(t_{i-1})}{t_i - t_{i-1}}, \text{ for some } t^* \in [t_i, t_{i+1}] \tag{13}$$

is derived, based on the mean-value theorem. A complete list of the equations and inequalities generated by Q2 is given by Kuipers (1994).

The equations and inequalities obtained for the qualitative behavior are used in the second step to constrain the interval bounds on the landmark values. Q2 transforms the landmarks, their interval bounds, and the equations and inequalities into a CSP, which is then solved by local constraint propagation based on interval arithmetic (Kuipers, 1994). The propagation of numerical information results into a *semi-quantitative behavior* refining the qualitative behavior, or leads to a refutation of the qualitative behavior (when the interval of a landmark value reduces to Ø). Although conceptually the propagation of numerical information takes place after generation of the complete behavior tree by QSIM, in practice Q2 is integrated with qualitative simulation and functions as a global constraint on the generation of new qualitative states at distinguished time-points. The single semi-quantitative behavior of a linear, undamped mass–spring system predicted by Q2 is shown in Figure 15 (Vatcheva, 2001). Using the intervals bounding the value of k and the initial value x_0 of the displacement, Q2 derives interval bounds for all landmark values in the qualitative behavior. For instance, the value of x at t_2, given by the landmark x_1, is predicted to lie in the interval $[-8.6, -8.3]$.

A problem with Q2 is that its predictions are rather weak due to the coarse time-step implied by the qualitative behavior. In fact, the time-step equals the difference between two consecutive distinguished time-points, as shown by Equation (13). Berleant and Kuipers (1992, 1997) have developed Q3, which adaptively refines the step size of Q2 by inserting new states into a qualitative behavior, and thus tighten the interval bounds on the landmark values.



	x_0	x_1	v_1	v_2	a_0
range	[8.3, 8.6]	[−8.6, −8.3]	[−3.04, −2.3]	[2.3, 3.04]	[−1.08, −0.638]

	a_1	t_1	t_2	t_3	t_4
range	[0.638, 1.08]	[2.73, ∞]	[5.46, ∞]	[8.19, ∞]	[10.9, ∞]

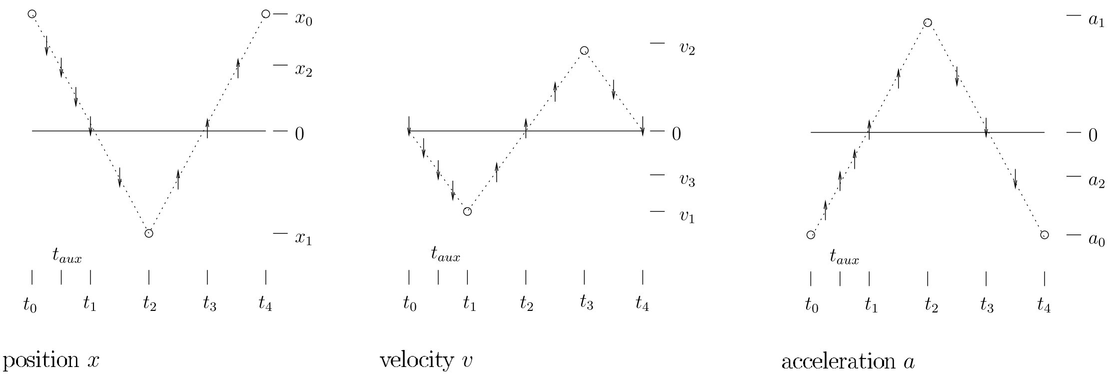
Figure 15 Semi-quantitative behavior obtained by applying Q2 in combination with QSIM to the mass-spring system (4)–(5), with *range* (k)=[0.08, 0.13], and initial conditions *range* (x_0)=[8.3, 8.6] and *range* (v_0)=[0, 0]. The table gives the intervals for the landmarks in the graph (Vatcheva, 2001)

In a first step, step-size refinement locates a *gap* in a semi-quantitative behavior produced by QSIM and Q2. A time-interval state $QS(t_i, t_{i+1})$ in the behavior represents a gap, if for the interval bounds on t_i and t_{i+1}, given by $[\underline{t}_i, \overline{t}_i]$ and $[\underline{t}_{i+1}, \overline{t}_{i+1}]$, respectively, it holds that $\overline{t}_i < \underline{t}_{i+1}$. An example of a gap in Figure 15 is the state between t_0 and t_1 (given that $t_0 \in [0, 0]$). If no gap exists, Q3 tries to create them by means of auxiliary techniques, called target interval partitioning and behavior splitting (Berleant & Kuipers, 1997).

In the next step, Q3 interpolates a new state in the gap at an auxiliary time-point t_{aux}, $\overline{t}_i < t_{\text{aux}} < \underline{t}_{i+1}$, where t_{aux} is assigned an exact numerical value (i.e., its value lies in an interval of zero width). The insertion of a new state is achieved by the creation of new landmarks and by updating the corresponding quantity spaces. The landmarks are initialized with interval bounds given by the union of the bounds of the corresponding landmarks at t_i and t_{i+1}. The newly-created landmarks add variables and constraints to the CSP. A new round of constraint propagation by means of Q2 may lead to a refinement of the interval bounds of the landmarks. In the example of Figure 15, the insertion of a new state at $t_{\text{aux}}=1.36$, in the gap between t_0 and t_1, leads to an improvement of the bounds on the value of the time landmarks. Thus, the interval for t_1 is refined from [2.73, ∞] to [3.44, 14.4], as shown in Figure 16. On the other hand, the interval bounds for the landmarks of the position, velocity, and acceleration of the mass remain unchanged in the example. The location of gaps and the interpolation of states are repeated until sufficiently precise results are obtained or no further refinements occur.

The extension of QSIM with Q2 and Q3 does not change the soundness of the simulation process. In fact, Q2 and Q3 have been shown to generate all genuine semi-quantitative behaviors of the system. That is, every real solution of an ODE consistent with the SQDE is included among the predictions of Q2 and Q3 (Kuipers, 1994). However, Q2 and Q3 are incomplete, in that they are not guaranteed to exclude all spurious semi-quantitative behaviors. The incompleteness of Q2 and Q3 is a consequence of the incompleteness of QSIM and the occurrence of excess width in interval computations (Moore, 1979). Q3 has the additional property that, given precise initial conditions, the width of the bounding intervals of the system variables will tend towards 0 as the step size of the simulation becomes infinitely small. This *convergence* property allows Q3 to bridge the gap between qualitative and numerical simulation.

The QSIM and Q2 programs are available at `http://www.cs.utexas.edu/users/qr/`, while a LISP implementation of Q3 has been developed by Vatcheva (2001). These programs have



	x_2	v_3	a_2
range	[6.8, 8.32]	[−1.47, −0.76]	[−1.08, −0.6]

	t_1	t_2	t_3	t_4
range	[3.44, 14.4]	[6.17, ∞]	[8.90, ∞]	[11.6, ∞]

Figure 16 Interpolation of an additional state at t_{aux}=1.36 in the gap between t_0 and t_1 (Figure 15). The following landmarks have been created: x_2, v_3, and a_2. The table gives the corresponding interval bounds and the refined interval bounds of the distinguished time-points (Vatcheva, 2001)

been used in various applications, such as the selection of experiments to efficiently discriminate between alternative semi-quantitative models of the growth of microorganisms in a chemostat (Figure 11). The predictions of the models allow the optimal discriminatory experiment(s) to be determined, using an entropy-based criterion that measures the expected informativeness of experiments (Vatcheva *et al*., 2000, 2001; Vatcheva, 2001). Model discrimination has been achieved in the presence of several complicating factors, in particular the complexity of the models, the large uncertainty in the parameter values, and the difficulty to observe the system behavior.

6 Discussion

Methods for qualitative simulation allow predictions to be made on the behavior of systems for which no quantitative information is available. In addition, they can be helpful when striving the comprehension of the range of possible qualitative behaviors compatible with the structure of the system. QSIM and other qualitative simulation methods, originally developed in the 1980s, and improved and extended since then, are able to predict the possible qualitative behaviors of a system, given a qualitative model and an initial qualitative state. The use of these methods in realistic scientific and engineering applications has revealed two serious problems. On the one hand, the predicted qualitative behaviors may be spurious, while on the other hand, their number may be so overwhelming as to render the results useless for practical purposes.

Two alternatives for qualitative simulation methods have been discussed in this review, addressing the above-mentioned problems in different ways. Qualitative phase-space analysis methods interpret qualitative simulation in the framework of dynamic systems theory. They usually focus on classes of systems for which strong mathematical constraints exist. By adapting the behavior representations and prediction algorithms to these constraints, they try to avoid spurious and uninformative behavior predictions. Semi-quantitative simulation methods augment the qualitative models with weak numerical information, in particular bounds on parameter values and functional relations. In many situations of practical interest, this information is available over and above purely qualitative information. The use of numerical information allows the semi-quantitative methods to reduce the number of qualitative behavior predictions and increase their precision. Qualitative phase-space analysis and semi-quantitative simulation have been used to analyze the behavior of large and complex systems, yielding results of scientific and technological relevance. Nevertheless, it has to be admitted that these approaches remain far less upscalable than

Table 4 Comparative evaluation of methods for qualitative simulation, qualitative phase-space analysis, and semi-quantitative simulation

	Qualitative simulation	Qualitative phase-space analysis	Semi-quantitative simulation
Mathematical foundation	Basic calculus	Dynamic systems theory	Numerical and interval analysis
Type of model	Qualitative	Qualitative or quantitative	Semi-quantitative
Genericity of method	High	Usually low, restricted to models with strongly constrained dynamics	High
Implementation	Yes	Some	Yes
Soundness	Yes	Some[1]	Some[1]
Spurious behaviors	Many	Some	Some
Upscalability	Low	Moderate	Moderate[2]
Realistic applications	Few	Yes	Yes

[1]Numerical phase-space analysis and interval simulation methods are often not sound.
[2]Upscalability depends on tightness of interval bounds.

numerical simulation. This is the price to be paid for the use qualitative or semi-quantitative models.

Qualitative simulation methods have been shaped by their origins in artificial intelligence, combining concepts from cognitive science with techniques from engineering mathematics. Qualitative phase-space analysis and semi-quantitative simulation, on the other hand, draw upon well-established concepts and techniques from other domains, such as dynamic systems theory, control theory, and interval analysis. Although the approaches discussed in this report often employ different languages and emphasize different aspects, it is clear that they share many basic intuitions. This is evident from the cross-fertilization that has occurred in the course of time. For example, the development of global constraints for QSIM has been largely inspired by results from dynamic systems theory. Some of the qualitative phase-space analysis methods mentioned in Section 4.1 have started as reformulations of the ideas underlying QSIM, retaining important concepts like qualitative state and qualitative state transition in the process. Furthermore, Q2 and Q3 have shown that the predictions of semi-quantitative simulation can be improved by using the qualitative behavior tree of QSIM as a scaffold for numerical calculations.

Qualitative simulation, qualitative phase-space analysis, and semi-quantitative simulation have different strengths: while qualitative simulation methods have a strong computational orientation, qualitative phase-space analysis and semi-quantitative simulation methods possess a solid foundation in dynamic systems theory and numerical analysis (see Table 4 for a synthesis and comparison). The review of these approaches in the preceding sections suggests that the respective strengths of the approaches could be profitably combined into a computational framework for the qualitative analysis of dynamic systems. This framework would provide a common conceptual basis for different methods, each tailored to a particular class of dynamic systems, while being flexible enough to apply to qualitative as well as (partially) quantitative models. The development of this synthetic framework could profit from work on the analysis of hybrid systems and control theory, where ideas similar in spirit to qualitative simulation have emerged (e.g. Lunze, 1994, 1998; Alur *et al.*, 2000; Asarin *et al.*, 2000, 2002; Aubin & Dordan, 2002; Tiwari & Khanna, 2002).

A synthetic computational view on the qualitative analysis of dynamic systems should establish a solid basis for achieving further upscaling, required for most real-life applications in science and engineering. Shults and Kuipers (1997) have started to explore one possible direction, consisting of the combination of qualitative simulation and techniques for *model checking* (Bérard *et al.*, 2001; Clarke *et al.*, 1999). Instead of explicitly generating a behavior tree, and then extracting appropriate information by visual inspection, the method proves temporal logic statements about the possible qualitative behaviors of the system under study. The merit of this approach, and related work in the same line (Kuipers & Åström, 1994; Brajnik & Clancy, 1996, 1998; Batt *et al*., 2004), is that it opens a perspective on the application of the huge body of techniques developed for the analysis of discrete-event systems. For instance, techniques developed to treat the state explosion problem in model checking might be profitably used for the qualitative analysis of dynamic systems.

Another way to proceed, complementary to a shift from the explicit generation of qualitative behaviors to the verification of behavorial properties, is to focus on the manner in which models are formulated in the first place. Instead of directly reflecting the size and complexity of the system in the model, one might try to decompose a system into subsystems, simulate each of these separately, and study the interactions between the subsystems on a higher level of abstraction. Model decomposition based on the degree of connectivity of system components, on the relative strength of their interactions, or on the hierarchy of time-scales of processes, is part of standard practice in mathematical modeling. Although important work on the integration of these modeling strategies with qualitative reasoning has been carried out (e.g. Kuipers, 1988; Iwasaki, 1992; Weld, 1992; Weld & Addanki, 1992; Iwasaki & Simon, 1994; Nayak, 1994; Rickel & Porter, 1994, 1997; Williams & Raiman, 1994; Yip, 1996; Clancy & Kuipers, 1997a, 1998; Sachenbacher & Struss, 2003), many issues remain to be explored.

Making predictions on the qualitative behavior of dynamic systems is usually not an isolated goal, but part of a broader task context, such as monitoring an industrial process, diagnosing a faulty device, or inferring the structure of an experimental system from its observed behavior. Future methods for the qualitative analysis of dynamic systems must therefore be integrated with other reasoning methods focusing on such tasks as model building, model testing, model discrimination, and model revision. Ultimately, this may result in versatile computer environments for the analysis of dynamic systems, like the computer-supported discovery environments envisioned in de Jong & Rip (1997) and the environment for nonlinear system identification explored in Bradley *et al*. (1998, 2001) and Bradley & Stolle (1996). A remarkable aspect of these applications will be their heterogeneous nature, in the sense that they will require the integration of techniques from mathematics, computer science, and logic.

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