Qualitative Simulation and Related Approaches for the Analysis of Dynamical Systems

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INRIA

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

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N° 5128

Fevrier 2003

THÈME 3

ISSN 0249-6399 ISRN INRIA/RR--5128--FR+ENG

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RHÔNE-ALPES

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Thème 3 — Interaction homme-machine,
images, données, connaissances
Projets HELIX

Rapport de recherche n° 5128 — Fevrier 2003 — 44 pages

Abstract: Methods for qualitative simulation allow predictions to be made on the behavior of a system for which no quantitative information is available. In addition, they help obtain a comprehension of the range of possible qualitative behaviors compatible with the structure of a system. This report 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 dynamical systems have emerged: qualitative phase space analysis and semi-quantitative simulation. The report argues for a synthesis of these approaches to obtain a computational framework for the qualitative analysis of dynamical systems. This should provide a solid basis for further upscaling and for the development of model-based reasoning applications of a wider scope.

Key-words: Qualitative reasoning, qualitative simulation, QSIM, qualitative analysis of dynamical systems, semi-quantitative simulation, interval simulation, modeling, Q2, Q3, loop-structured systems

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Simulation qualitative et des approches liées pour l'analyse de systèmes dynamiques

Résumé : Les méthodes pour la simulation qualitative permettent de faire des prédictions du comportement d'un système donné quand aucunes informations quantitatives ne sont disponibles. En outre, elles aident à obtenir une compréhension des comportements qualitatifs possibles permis par la structure d'un système. Ce rapport fait une synthèse de QSIM et d'autres méthodes de simulation qualitative. Il traite deux problèmes qui ont sérieusement compromis l'application de ces méthodes à des problèmes scientifiques et technologiques réalistes : l'existence de prédictions de comportements factices, ainsi que l'explosion combinatoire du nombre de prédictions de comportements. En réponse à ces problèmes, d'autres approches pour l'analyse qualitative de systèmes dynamiques ont émergé : l'analyse qualitative de l'espace de phase et la simulation semi-quantitative. Le rapport prône une synthèse de ces approches afin d'obtenir un cadre algorithmique pour l'analyse qualitative de systèmes dynamiques. Ceci devrait jeter une base solide permettant la mise à l'échelle de la simulation qualitative et le développement des applications plus larges du raisonnement à partir de modèles.

Mots-clés : Raisonnement qualitatif, simulation qualitative, QSIM, analyse qualitative de systèmes dynamiques, simulation semi-quantitative, simulation d'intervalles, modélisation, Q2, Q3, systèmes en boucles

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 one reaction occurs faster than another. 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 aim as 'formalizing common-sense reasoning' or 'doing qualitative physics' (*e.g.*, [51, 67, 85, 119]). 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 has 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 [53, 54] (see also [197]), the process-based approach of Forbus [68, 75], and the constraint-based approach of Kuipers [108, 114, 110]. 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 [23, 195] for collections of papers at the origin of the above methods and [72, 113, 112, 201] for retrospectives).

In the ENVISION approach of de Kleer and Brown [53, 54], 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 [68, 75] 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' *QSIM* approach [108, 110, 114] has focussed 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 is 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 approach towards qualitative simulation. Its clear definition of concepts like qualitative model, qualitative state and behavior, and its explicit relation between qualitative and numerical simulation, has 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. ENVISION and QPT have exerted a considerable 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 [22, 25, 102, 134]. As a further contribution of ENVISION, one may 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 [196, 200] and the order-of-magnitude calculus of Raiman [148]. The process-centered ontology of QPT lies at the root of a number of model composition techniques (*e.g.*, [63, 65, 124, 126, 136, 151], reviewed in [107, 166, 203]).

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 [64, 195] and the proceedings of the annual *International Workshop on Qualitative Reasoning* for collections of papers). 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 medecine, biology, and ecology.

After the initial heydays in the eighties and early nineties, 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 upscale 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 dynamical systems theory, control theory, and interval analysis. By tailoring the method to classes of dynamical 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. It builds upon earlier reviews on qualitative simulation, such as the chapter introductions in [195], the QSIM book of Kuipers [114], recent book chapters by Forbus and Kuipers [73, 115], and an extensive review on qualitative reasoning

by the MQ&D author collective [41] (see also [52, 70, 110]). An excellent review placing qualitative simulation in the wider context of model-based reasoning is available in German [176]. A new edition of a French textbook on qualitative reasoning [179], with chapters on many of the topics discussed in this report, recently appeared. The critical discussion of qualitative simulation by Doyle and Sacks [160] 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 the sections 4 and 5, respectively. The review finishes with a discussion of some perspectives for qualitative simulation.

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^{++}).

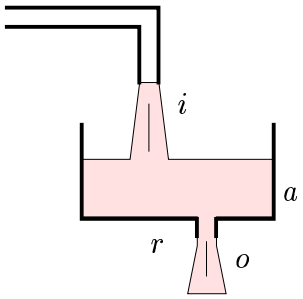


Figure 1: Simple tank system. The variables have the following interpretation: a water amount, r area of orifice, i inflow, o outflow. r and i are constants

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 the differential equation (section 2.2). The computation of qualitative states and state transitions is determined by 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 [108] and the textbook [114]. For more details the reader is referred to these sources.

2.1 Qualitative values, states ,and behaviors

QSIM considers the variables $\boldsymbol{v} : [a, b] \rightarrow (\mathbb{R}^*)^m$ of a dynamical 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 [114]. $-\infty$, 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 $\langle qmag, qdir \rangle$, 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 $\boldsymbol{v}$ at t. For example, the area r of the orifice at t_0 is represented by the qualitative value $QV(r,t_0) = \langle max, std \rangle$. Since r is a constant, it will have the same qualitative value at a later time-point: $QV(r,t_1) = \langle max, std \rangle$. If the orifice is only partially opened, then the qualitative value of its area, $QV(r,t_0)$, equals $\langle]0, max[, std \rangle$ (*idem* for later time-points).

The *qualitative value of a variable v on a time-interval* $]t_i, t_{i+1}[$ follows from the qualitative value at the time-points in the interval. If t_i and t_{i+1} are adjacent distinguished time-points, 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 $t \in]t_i, t_{i+1}[$. 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 $QV(a, t_0, t_1) = \langle]0, \infty[, inc \rangle$.

A *qualitative state* of a dynamical 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 $\boldsymbol{v}$:

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

where t_i and t_{i+1} are distinguished time-points of some variable v_j, $1 \leq j \leq m$.

The *qualitative behavior* of a dynamical system with variables $\boldsymbol{v}$ on $[a,b]$ is the sequence of qualitative states

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

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. In general, a qualitative behavior will be satisfied by a class of reasonable functions.

2.2 Qualitative differential equations

QSIM models dynamical systems by means of *qualitative differential equations (QDEs)*. A QDE is an abstraction of an ordinary differential equation (ODE), usually written in the from 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 $f_i : \Omega \rightarrow \mathbb{R}^*$, $1 \leq i \leq n$, 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) may be composed of functions that are incompletely specified, in the sense that they are only specified as belonging to a certain monotonicity class. Kuipers [114] lists a number of monotonicity classes. M^+ is the class of monotonically increasing functions, that 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 element f 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 $z = f(x, y)$, such that $\partial f/\partial x > 0$ and $\partial f/\partial y > 0$ over the domain of the function f.

More precisely, 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 $\boldsymbol{v}$, include the state variables $\boldsymbol{x}$ and the parameters $\boldsymbol{p}$, but also any auxiliary variables introduced through the reduction of the ODE to basic equations.

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)	$z(t) = y(t)\,x(t)$
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$^{++}(x, y, z)$	$z(t) = f(y(t), x(t)),\ f \in M^{++}$

Table 1: Qualitative constraints and the basic mathematical equations of which they are abstractions. Analogous constraints for subtraction ($-$), division ($/$), monotonically decreasing functions (M^-, M_0^-), and other multivariate monotonic functions (M^{--}, M^{+-}, M^{-+}) have been omitted.

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

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

(a) (b)

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.

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).

2.3 Constraints on qualitative values

The computation of qualitative states and state transitions is determined by three types of constraints on 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 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 $\langle qmag_x, qdir_x\rangle$, $\langle qmag_y, qdir_y\rangle$, and $\langle qmag_z, qdir_z\rangle$ 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 $qval_x = \langle]0, \infty[, \mathit{inc}\rangle$ and $qval_y = \langle 0, \mathit{std}\rangle$, then necessarily $qval_z = \langle]0, \infty[, \mathit{inc}\rangle$.

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

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

Table 2: Definition of the ADD constraint. A question mark means that the qualitative magnitude (direction) of z can be any of $]-\infty, 0[$, 0, or $]0, \infty[$ (*dec*, *std*, or *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), and $qmag_x =]-\infty, 0[$, $qmag_y =]0, \infty[$, 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 $\langle l_x, l_y, l_z \rangle$ is a corresponding value triple for the ADD constraint. Given that $qmag_x =]l_x, \infty[$ and $qmag_y = l_y$, then we can immediately infer that $qmag_z =]l_z, \infty[$. In order to formalize the state constraints in an appropriate and general way, Kuipers [114] uses the sign-real algebra of Williams [200].

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 [170] 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 from one qualitative value to the next for a continuously differentiable function $v : [a, b] \to \mathbb{R}^*$, where $l_{j-1} < l_j < l_{j+1}$ are three adjacent landmarks in the quantity space of v.

P-transitions

$QV(v, t_i)$	$\Rightarrow$	$QV(v, t_i, t_{i+1})$
$\langle l_j, std \rangle$		$\langle l_j, std \rangle$
$\langle l_j, std \rangle$		$\langle]l_j, l_{j+1}[, inc \rangle$
$\langle l_j, std \rangle$		$\langle]l_{j-1}, l_j[, dec \rangle$
$\langle l_j, inc \rangle$		$\langle]l_j, l_{j+1}[, inc \rangle$
$\langle l_j, dec \rangle$		$\langle]l_{j-1}, l_j[, dec \rangle$
$\langle]l_j, l_{j+1}[, inc \rangle$		$\langle]l_j, l_{j+1}[, inc \rangle$
$\langle]l_j, l_{j+1}[, dec \rangle$		$\langle]l_j, l_{j+1}[, dec \rangle$
$\langle]l_j, l_{j+1}[, std \rangle$		$\langle]l_j, l_{j+1}[, std \rangle$
$\langle]l_j, l_{j+1}[, std \rangle$		$\langle]l_j, l_{j+1}[, inc \rangle$
$\langle]l_j, l_{j+1}[, std \rangle$		$\langle]l_j, l_{j+1}[, dec \rangle$

I-transitions

$QV(v, t_i, t_{i+1})$	$\Rightarrow$	$QV(v, t_{i+1})$
$\langle l_j, std \rangle$		$\langle l_j, std \rangle$
$\langle]l_j, l_{j+1}[, inc \rangle$		$\langle l_{j+1}, std \rangle$
$\langle]l_j, l_{j+1}[, inc \rangle$		$\langle l_{j+1}, inc \rangle$
$\langle]l_j, l_{j+1}[, inc \rangle$		$\langle]l_j, l_{j+1}[, inc \rangle$
$\langle]l_j, l_{j+1}[, inc \rangle$		$\langle]l_j, l_{j+1}[, std \rangle$
$\langle]l_j, l_{j+1}[, dec \rangle$		$\langle l_j, std \rangle$
$\langle]l_j, l_{j+1}[, dec \rangle$		$\langle l_j, dec \rangle$
$\langle]l_j, l_{j+1}[, dec \rangle$		$\langle]l_j, l_{j+1}[, dec \rangle$
$\langle]l_j, l_{j+1}[, dec \rangle$		$\langle]l_j, l_{j+1}[, std \rangle$
$\langle]l_j, l_{j+1}[, std \rangle$		$\langle]l_j, l_{j+1}[, std \rangle$

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

[1] For a generalization of the definition of corresponding values, based on the use of intervals with landmark value bounds, see [163].

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.

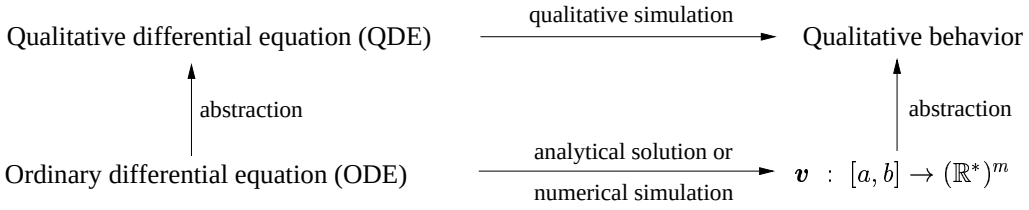


Figure 3: Abstraction relations in qualitative simulation.

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 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, signalizing 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 leaves of a tree, that is, from the initial state(s) to states without successors. Given a QDE with variables $\boldsymbol{v}$ 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 leaves 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.

This 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 [114] 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 [66]. 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 which check consistency of the states with the various types of qualitative constraints. 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:

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

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 the steps 2 to 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 part (b)-(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] Other implementations of QSIM, in Prolog and in C++, are described in [11, 62]. For implementations of QPT, see [71, 75].

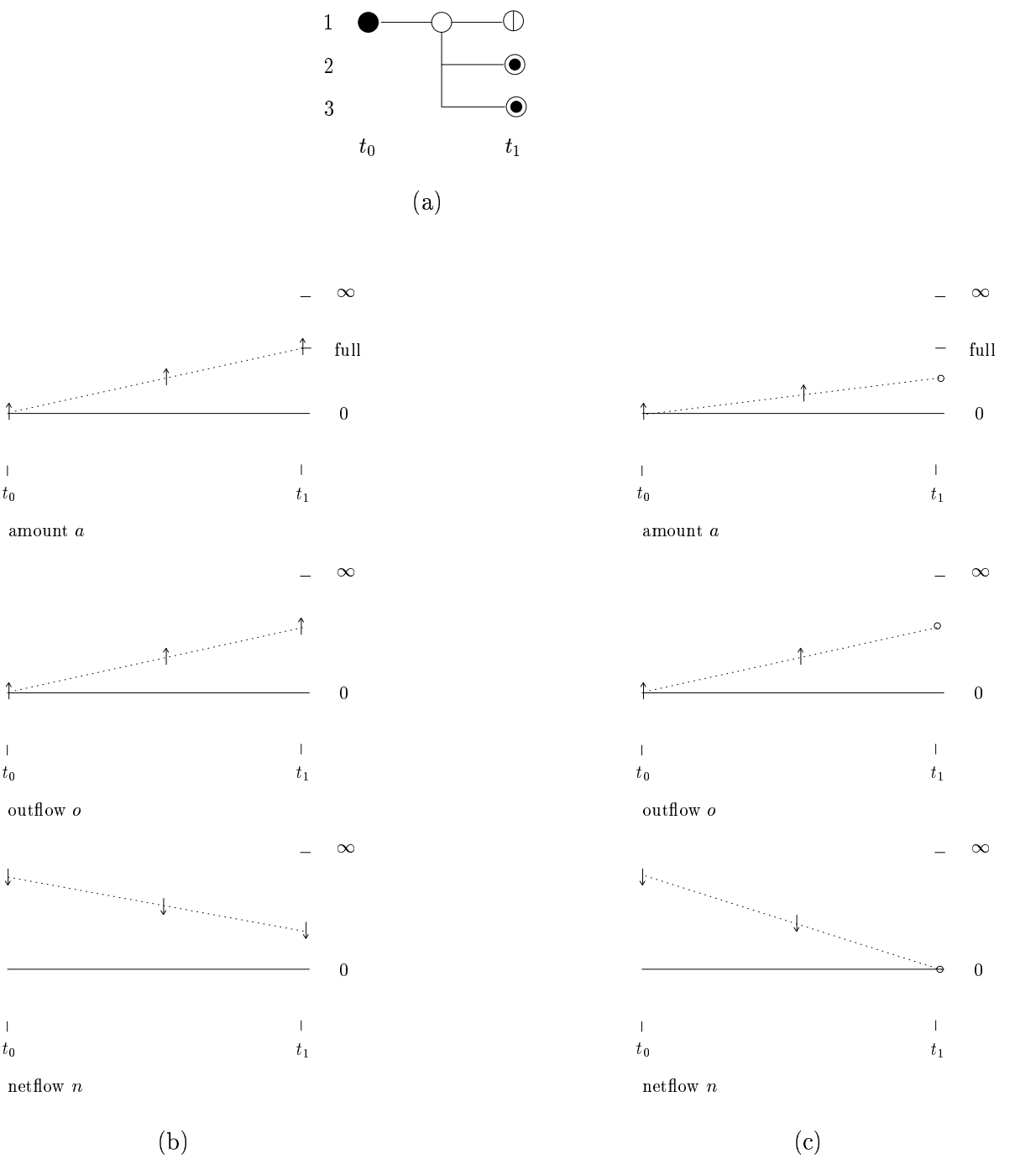


Figure 4: (a) Qualitative behavior tree for the simple tank system in figure 1. (b)-(c) The temporel evolution of a few distinctive variables according to the qualitative behaviors 1 and 3. The notation is as follows: • denotes a qualitative state at a time-point, ∘ a qualitative state over a time-interval, ◉ a quiescent state, ⓘ a transition state, and ◎ the end of a period. The symbols ↑, ↓, and ∘ in the graphs refer to increasing, decreasing, and steady directions, respectively [66].

2.5 Properties of qualitative simulation

A productive way to look at QSIM 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 $QB_1 \vee \ldots \vee QB_l$.

QSIM is *sound* and *incomplete* in that the disjunction of possible qualitative behaviors contains all genuine behaviors of the system, but occasionally spurious behaviors as well. A *spurious* qualitative behavior QB is a qualitative behavior which describes no solution to any initial value problem ODE and $\boldsymbol{v}(t_0) = \boldsymbol{v_0}$ satisfying QDE and $QS(init)$. A well-known example of a spurious qualitative behavior is the mass-spring behavior violating the law of energy conservation [114], which will be discussed in section 3.1. A non-spurious behavior is called a *genuine* qualitative behavior. In the case of a spurious qualitative behavior, the behavioral abstraction relation in figure 3 breaks down.

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 [108]. What is more, the algorithm need not halt and can continue producing ever more and ever longer qualitative behaviors.

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.

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), as well as 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 situations 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.

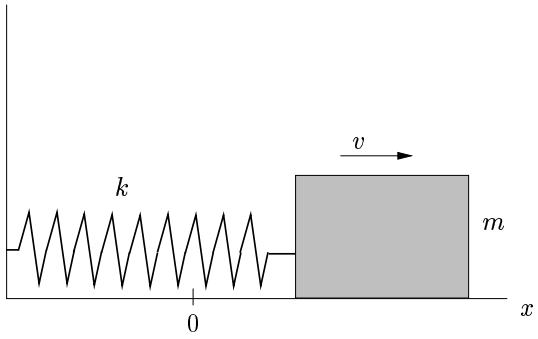


Figure 5: Undamped mass-spring system. The variables refer to the position x, velocity v, acceleration a, and mass m of the block, as well as the spring constant k.

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 variables. Since 1 and -1 are roots of (3), in addition to 0, we insert landmark values corresponding to these numbers in the quantity spaces of the variables. Furthermore, appropriate corresponding value triples are defined for the constraints (not shown).

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)
(a)	(b)

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

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 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 ([132]; see [174] 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.

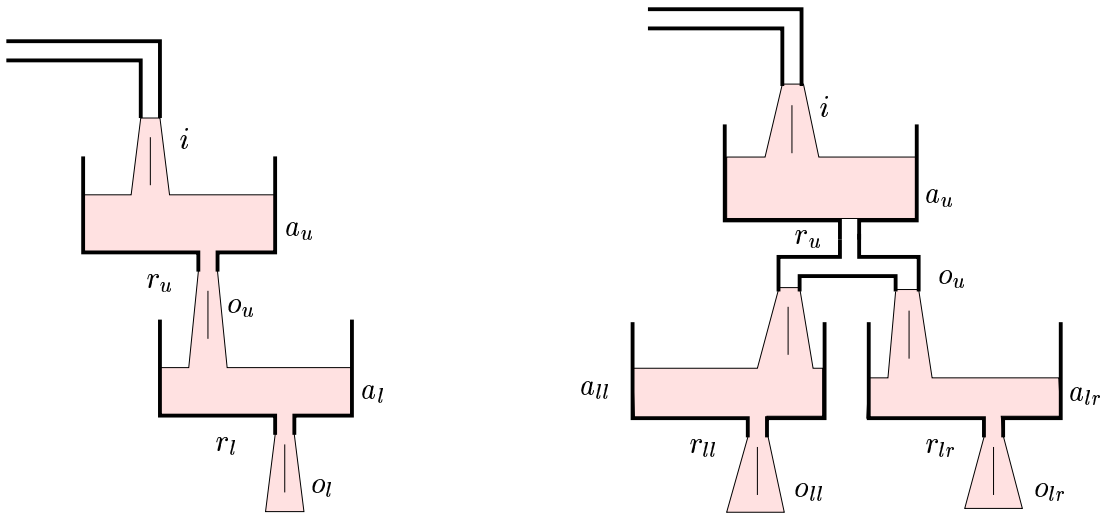


Figure 7: Two cascaded-tanks system. The variable names have the following interpretation: a water amount, r area of orifice, i inflow, o outflow. r and i are constants. The subscripts $\cdot_u$ and $\cdot_l$ refer to the upper and lower tanks, respectively, while $\cdot_{ll}$ and $\cdot_{lr}$ denote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

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 $QV(n_l, t_0) = \langle]0, \infty[, inc \rangle$. The initial qualitative state

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) quantity spaces of variables and (b) qualitative constraints.

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, $QV(n_l, t_0, t_1) = \langle]0, \infty[, inc \rangle$. 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 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 focussing 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 [114, 118]. 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. Hussain and Ray have generalized the qualitative state description and transition table to take into account second-order time derivatives [89]. This work builds upon earlier ideas on the use of higher-order time derivatives in qualitative simulation, such as [53, 198].

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:

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

$$\dot{v} = -k\,x. \tag{5}$$

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.

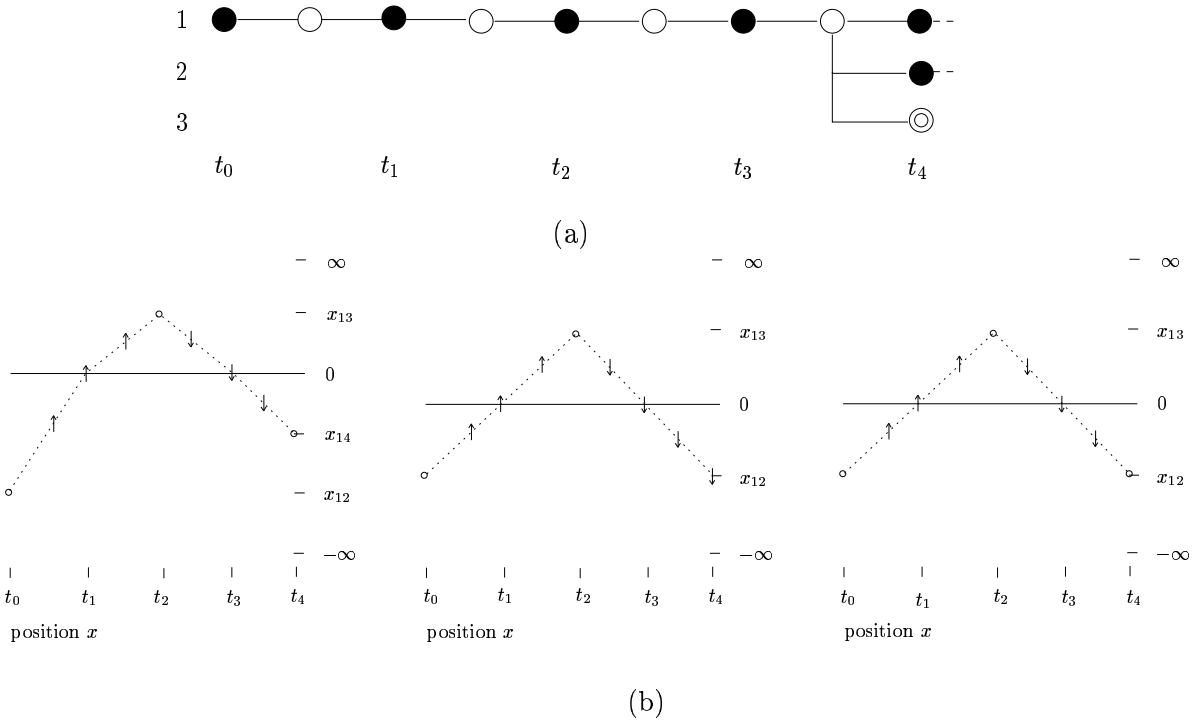


Figure 9: (a) Qualitative behavior tree for the undamped mass-spring system (see figure 4 for the notation). (b) The temporal evolution of the position x of the spring in the three behaviors.

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

$$E = \frac{1}{2}\,m\,v^2 + \frac{1}{2}\,k\,x^2$$

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 dynamical systems theory (section 4). Examples of global constraints include energy constraints, or more generally Lyapunov functions [79, 88], non-intersection constraints on trajectories in the phase space [121, 173], constraints on qualitative stability and instability [92], constraints based on l'Hôpital's rule [161], and analytical function constraints [118].

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:

$$\begin{aligned}
\dot{a}_u &= i - f(a_u, r_u),\ f \in M^{++},\\
\dot{a}_{ll} &= f(a_u, r_u) - g(a_{ll}, r_{ll}),\ g \in M^{++},\\
\dot{a}_{lr} &= f(a_u, r_u) - h(a_{lr}, r_{lr}),\ h \in M^{++},
\end{aligned}$$

where the variables i, a, and r have the same meaning as before, and the suffixes $\cdot_{ll}$ and $\cdot_{lr}$ 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* [178]. 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 in 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 [38, 40, 68, 199] or the reduction of qualitative behavior trees by compacting several qualitative behaviors into a single abstract qualitative behavior [62, 130, 178, 189].

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 [114, 117]. An example of chattering occurs in a damped mass-spring system given by:

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

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

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, in a qualitative state in which x is positive and *inc*, and v positive and *dec*, repeated transitions to and from a qualitative state with

$QV(a) = \langle]-\infty, 0[, std \rangle$ occur.[3] Clancy and Kuipers [37] 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 [90, 91, 111, 151], (bio)chemical reactors [131, 182, 188] and chemical plants [35], digital circuits [103], fatigue and fracture in steel bridges [153], and genetic and ecological networks [82, 83, 86]. Moreover, QSIM and its relatives have been embedded in broader reasoning tasks, such as monitoring and diagnosis [56, 60, 61, 69, 120, 133, 140, 146, 147, 154, 155, 175, 188], model composition [63, 65, 124, 126, 136, 151], system identification [12, 30, 34, 84, 149, 164, 169, 181], theory refinement and measurement analysis [46, 101], tutoring [55, 74], and comparative analysis [50, 139, 190, 191, 192, 193].

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 [162]. 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 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 classes of behaviors known to be spurious. 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 [129, 158, 160]. 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 scalability 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.

[3] 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.

We conclude that the occurence 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 dynamical systems theory, in order to optimally exploit mathematical techniques available for certain classes of dynamical 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 on the behavior of large and complex systems.

4 Qualitative phase space analysis

4.1 Overview

Dynamical systems theory is a branch of mathematics that has developed powerful techniques for the qualitative analysis of dynamical systems [81, 87, 172]. 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. Changes in parameter values may lead to bifurcations, that is, to changes in the number or character of the attractors. Probably the best-known result of dynamical 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

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

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

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

Since the real part of the eigenvalues is negative, the equilibrium point is stable. If $\mu^2 > 4\,k$, then the eigenvalues are real, and an initial displacement is followed by an overdamped return to the equilibrium. On the other hand, if $\mu^2 < 4\,k$, then the eigenvalues have a real and an imaginary part, and the system oscillates back towards the equilibrium in an asymptotic manner.[4] 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 [171] 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 [79, 114] that are cumbersome to express in the QDE formalism, as well as mechanisms to detect and eliminate chattering variables. 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).

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

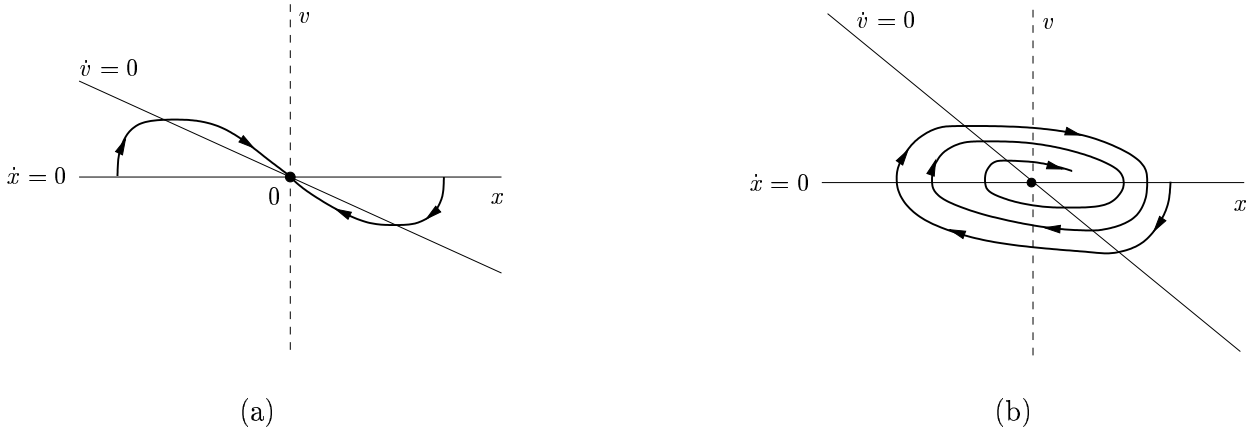


Figure 10: Example solution trajectories of the damped mass-spring system, for (a) $\mu^2 > 4\,k$ and (b) $\mu^2 < 4\,k$.

Reformulations of the QSIM approach in the framework of dynamical systems theory [8, 57, 122, 158] 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 dynamical system are weaker than those obtained by techniques developed in dynamical systems theory. Besides being a touchstone for the critical evaluation of work on qualitative simulation, the perspective of dynamical systems theory also provides a basis for the development of alternative methods [2, 100, 158]. Several such *qualitative phase space analysis* methods have been proposed since the early nineties. Contrary to QSIM and its relatives, these methods are tailored to a particular class of dynamical systems, in order to optimally exploit mathematical results 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, structured by means of concepts like equilibrium point, limit cycle, stability, and bifurcation. In comparison with well-known mathematical problem solvers like Maple, Mathematica, and Matlab, the phase space analysis programs add a layer of knowledge representation and task control that allows the coordinated application of a range of low-level numerical routines. A disadvantage of the methods is that a soundness guarantee like in QSIM cannot be given.

Examples of implemented numerical phase space analysis methods are KAM [204, 205], MAPS [210, 211], POINCARE [159], and PSX2NL [143]. 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 [27], MAPS has been used for nonlinear control design [31]. PSX2NL is a program for the generation of *flow patterns*, qualitative phase space structure descriptions, for planar ODEs. The method is based on a grammatical specification of all possible patterns of solution trajectories in the phase plane, which

confers it a certain robustness in the face of incomplete information and numerical error (see [141, 142, 144] for results obtained with relatives and extensions of PSX2NL). POINCARE is a numerical phase space analysis programs which analyzes one-parameter planar ODEs (see [1] for a precursor). It partitions the parameter interval into open subintervals with qualitatively homogeneous dynamics bounded by bifurcation points, and it constructs representative phase space structure descriptions for each subinterval. POINCARE has corrected the published analysis of a complex nonlinear reactor system in chemical engineering.

The models accepted 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 [17, 20], which will be discussed in more detail in section 4.2. It derives the qualitative transient and asymptotic behavior of loop-structured systems with monotonous 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 [157]. 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 [156]. Another example is the method of Dordan [57, 58], which is a reformulation of QSIM for so-called replicator systems, used in chemistry and ecology. De Jong and colleagues [44, 45, 47, 48] 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 [42, 43]. 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.[5] 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.

4.2 Qualitative analysis of loop-structured systems

Bernard and Gouzé have developed a method for the qualitative analysis of *loop-structured systems* with monotonous interactions [17, 20]. Examples of loop-structured systems, frequently occuring 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 $f_i : \Omega \to \mathbb{R}$ 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. The Jacobian matrix M of loop-structured systems has the following structure:

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

where $m_{ij} = \dfrac{\partial}{\partial x_j} f_i(\boldsymbol{x})$. Note that every two-dimensional system is by definition loop-structured. A loop-structured system is said to have *monotonous interactions* on Ω, if m_{ij}, $i \neq j$, does not change sign on Ω. The discussion below is restricted to loop-structured systems with monotonous interactions.

[5] Although not directly based on dynamical systems theory, the methods in [34, 165] are similar in spirit, in that they attempt to exploit the properties of a particular class of systems.

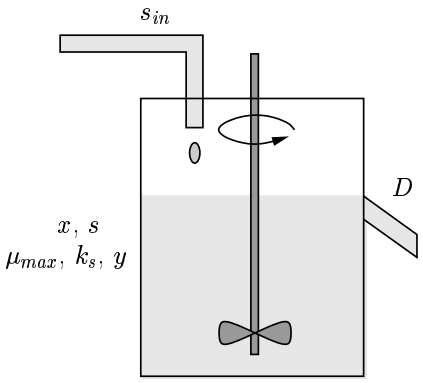


Figure 11: Schematic view of a chemostat. The variables denote the total amount x of biomass per unit volume and the concentration s of remaining nutrient. The parameters are the dilution rate D, the input nutrient concentration s_{in}, the maximum growth rate μ_{max} of cells, a half-saturation constant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

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*:

$$\dot{x} = \mu(s)\, x - D\, x, \tag{10}$$
$$\dot{s} = D\,(s_{in} - s) - \rho(s)\, x, \tag{11}$$

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 ($D > 0$, $s_{in} > 0$). The functions $\mu(s)$ and $\rho(s)$ are defined as follows:

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

with μ_{max} the maximum growth rate of cells, k_s a half-saturation constant, and y the growth yield ($\mu_{max} > 0$, $k_s > 0$, $y > 0$). The system described by the Monod model has monotonous 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

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

The hyperplanes associated with $\boldsymbol{x}^*$ divide the phase space into 2^n so-called $\boldsymbol{x}^*$*-orthants* $W_k(\boldsymbol{x}^*)$, $1 \le k \le 2^n$. In each $\boldsymbol{x}^*$-orthant, the sign of the difference $x_i - x_i^*$ is constant. The system is called *diagonally* $\boldsymbol{x}^*$*-monotonous*, 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 the single equilibrium point in Ω, denoted by (x^*, s^*) [16]. As can be easily verified, the Monod system is diagonally monotonous with respect to this equilibrium.

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

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

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.

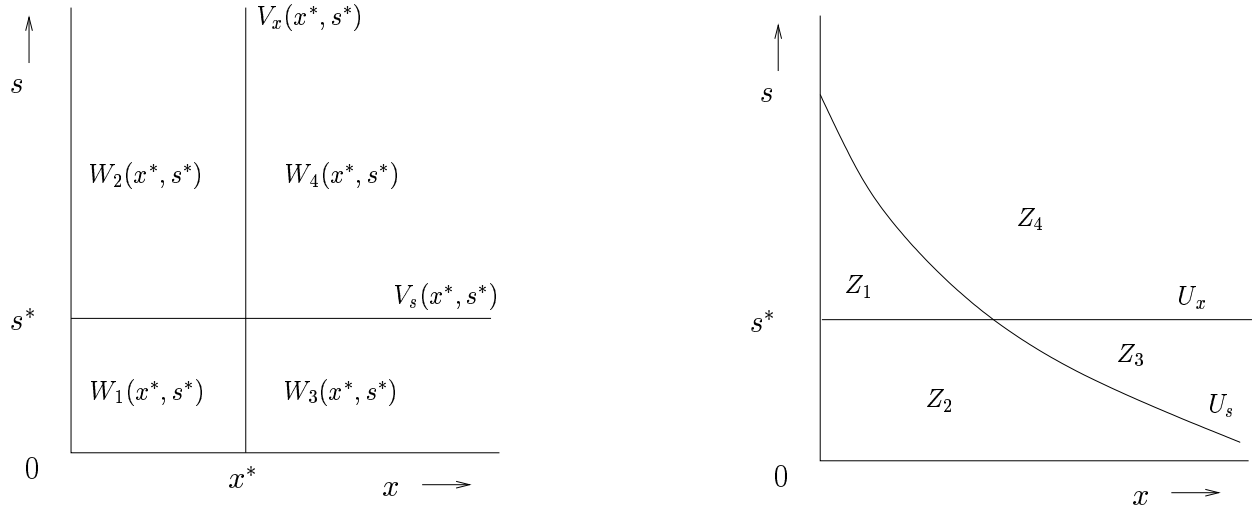


Figure 12: Subdivision of the phase space of the chemostat system in figure 11, described by the Monod model, into (a) $\boldsymbol{x}^*$-orthants and (b) z-orthants. $V_s(x^*, s^*) = \{(x, s) \in \Omega \mid s = s^*\}$, $V_x(x^*, s^*) = \{(x, s) \in \Omega \mid x = x^*\}$, $U_s = \{(x, s) \in \Omega \mid \dot{s} = 0\}$, and $U_x = \{(x, s) \in \Omega \mid \dot{x} = 0\}$. Furthermore, $Z_1 = \{(x, s) \in \Omega \mid \dot{x} > 0, \dot{s} > 0\}$, $Z_2 = \{(x, s) \in \Omega \mid \dot{x} < 0, \dot{s} > 0\}$, $Z_3 = \{(x, s) \in \Omega \mid \dot{x} < 0, \dot{s} < 0\}$, and $Z_4 = \{(x, s) \in \Omega \mid \dot{x} > 0, \dot{s} < 0\}$.

The computation of the possible qualitative states of a diagonally-monotonous loop-structured system amounts to determining, for each $\boldsymbol{x}^*$-orthant $W_k(\boldsymbol{x}^*)$, the z-orthants Z_l that it is compatible with. This is achieved by the theorems in [20], which express these compatibility relations in terms of the signs of the elements of the Jacobian matrix M. The possible transitions between the qualitative states can also be determined from the sign properties of M. In fact, criteria can be formulated 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) [20]. 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 results of a qualitative analysis can be visualized in the form of a *transition graph* (also called an *envisionment* in qualitative simulation). Each state is represented by a $n \times 2$-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 can be refined by taking into account the additional variable $u = s + (x/y)$, denoting the total nutrient concentration in the chemostat. It is easy to check that

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

The initial value u_0 of u puts additional restrictions on the possible behaviors allowed by the Monod model [16]. If $u_0 < s_{in}$, then $\dot{u}$ is positive, and hence x and s cannot simultaneously decrease. Moreover, if $\dot{u}$ is positive, then u is below its equilibrium value, and x and s cannot simultaneously be above their equilibrium value. On the other hand, if $u_0 > s_{in}$, then $\dot{u}$ is negative, and x and s cannot simultaneously increase. Moreover, if $\dot{u}$ is negative, then u is above its equilibrium value, and x and s cannot simultaneously be below their equilibrium value. The refined transition graph is shown in figure 13(b). For both $\dot{u} > 0$ and $\dot{u} < 0$ 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 state is based on a decomposition of the phase space that is more appropriate from a mathematical point of view. In addition, the computation of qualitative states and state transitions has been tailored to the loop-structured systems under study. This reduces the risk of generating uninformative or spurious qualitative states and state transitions. Theorems similar to the soundness property of QSIM (section 2.5) have been derived for the qualitative analysis of loop-structured systems [17]. The chemostat example concerns a two-dimensional system, but the method applies to loop-structured systems of dimension n.

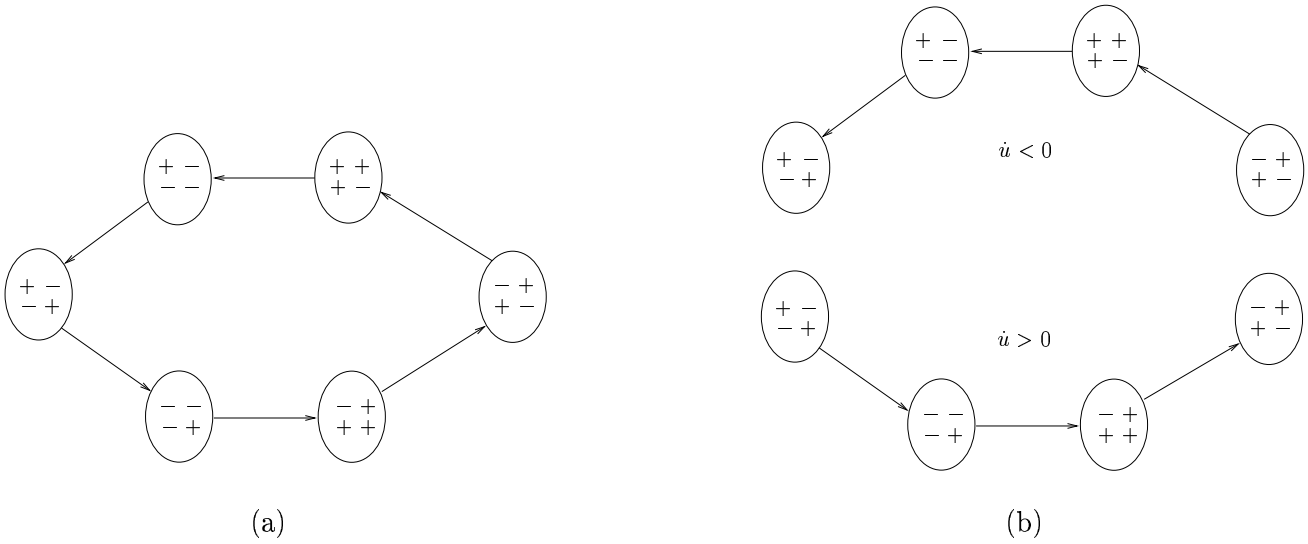


Figure 13: Transition graphs derived for the Monod model [16]. In (a) the variable u for the total nutrient concentration is not taken into account, whereas in (b) it is, leading to a refined transition graph. The first column in the sign matrix characterizing a state gives the position of the variables 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.

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 [17, 18, 19, 21]. 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 [19]. 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 the two extremes. In fact, for many scientific and engineering problems, numerical bounds on parameter values and functional relationships are available. This information can be exploited to arrive at better predictions than those obtainable through qualitative simulation alone. Several methods for *semi-quantitative* (or *semi-qualitative*) *simulation* have been proposed in the literature, based on a generalization of conventional numerical techniques by means of interval analysis [132]. More specifically, these methods deal with semi-quantitative models in which parameter values and initial conditions are specified by numerical intervals. In addition, functional relationships are sometimes defined by means of numerical envelopes.

In order to illustrate that numerical information, even of a weak nature, can refine the results obtained by qualitative methods, consider 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 numerical bounds on the value of k and μ are available, *i.e.* $k \in [0.001, 0.002]$ and $\mu \in [0.1, 0.3]$. From interval analysis it follows that $4\,k \in [0.004, 0.008]$ and $\mu^2 \in [0.01, 0.09]$, and hence $4\,k < \mu^2$. This excludes one of the behavioral possibilities, the oscillation of the mass around the equilibrium position. The use of intervals allows numerical uncertainty to be represented in a flexible way. 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, and thus constitutes a unifying framework for the representation of both qualitative and quantitative information.

Some semi-quantitative simulation methods, which will be called *qualitative-quantitative* methods, use the 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 [59, 80, 123]. The most well-known qualitative-quantitative methods are Q2, Q3, and NSIM. Q2 [14, 114] 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 [15] 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 more detail below. Q2 and Q3 can be used in combination with NSIM [105], which computes numerical envelopes for the solutions of a semi-quantitative model. Q2 and NSIM have been integrated into the simulator SQSIM [104]. The above extensions of QSIM have been used applied in model-based reasoning tasks like monitoring [61, 152], system identification [106], comparative analysis [184], and experiment selection [183, 185].

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 [132], a variety of such *interval simulation* methods have been proposed (*e.g.*, [97, 125, 137, 186]; see [5, 96, 138] for recent reviews).[6] The methods provide more 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 [125], 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, Delville, and Van Hentenrijck [97, 98]

[6] Similar methods for semi-quantitative simulation have been developed in the context of fuzzy simulation [24, 26, 167].

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 [187] and a gas turbine in a chemical plant [180].

In comparison with QSIM and its numerical extensions, interval simulation produces quantiative 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 [4, 76, 77, 78, 94]. 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 [74] 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 [10, 145, 206, 208, 209] (see [99] 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 [145]. 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 [14, 15, 114]. Q2 and Q3 assume that the system being considered is described by 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 $\mathit{range}(l) = [\underline{l}, \overline{l}]$, where $\underline{l}, \overline{l} \in \mathbb{R}^*$ and $\underline{l} \leq l \leq \overline{l}$. A bounding envelope for f is defined by $\mathit{envelope}(f) = [\underline{f}, \overline{f}]$, such that for all x in the domain of the function, it holds that $\underline{f}(x) \leq f(x) \leq \overline{f}(x)$. 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

$$\begin{aligned} \dot{x} &= v, \\ \dot{v} &= -k\, f(x),\ f \in M_0^+. \end{aligned}$$

The differential equations 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 $QS(t_0), QS(t_0, t_1), QS(t_1), \ldots, QS(t_p)$, Q2 first derives equations and inequalities, involving the landmarks of the system variables, from the qualitative values in $QS(t_i)$, $1 \leq i \leq p$, 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 $\mathrm{MULT}(x, y, z)$ leads to the equation $x(t_i)\, y(t_i) = z(t_i)$, while the monotonic

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

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.

function constraint $\mathrm{M}^+(x, y)$, for which the envelope functions $\underline{f}$ and $\overline{f}$ have been defined, gives rise to the inequalities $\underline{f}(x(t_i)) \leq x(t_i) \leq \overline{f}(x(t_i))$. Also, for the derivative constraint D/DT(x, y) the equality

$$\exists t^* : x(t^*) = \frac{y(t_i) - y(t_{i-1})}{t_i - t_{i-1}} \tag{13}$$

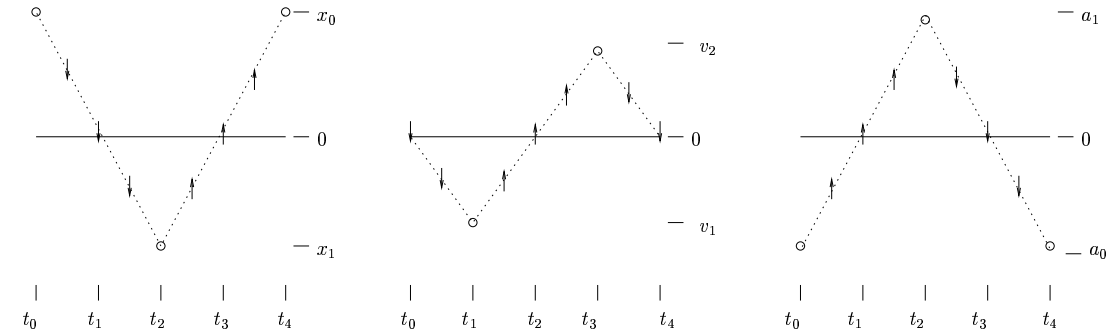
is derived, based on the mean-value theorem. A complete list of the equations and inequalities generated by Q2 is given by Kuipers [114].

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 [114]. 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 $\emptyset$). 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 [182]. 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 [14, 15] have developed Q3, which adaptively refines the step size of Q2 by inserting new states in a qualitative behavior, and thus tighten the interval bounds on the landmark values.

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, target interval partitioning and behavior splitting [15].

In the next step, Q3 interpolates a new state in the gap at an auxiliary time-point t_{aux}, $\overline{t}_i < t_{aux} < \underline{t}_{i+1}$, 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

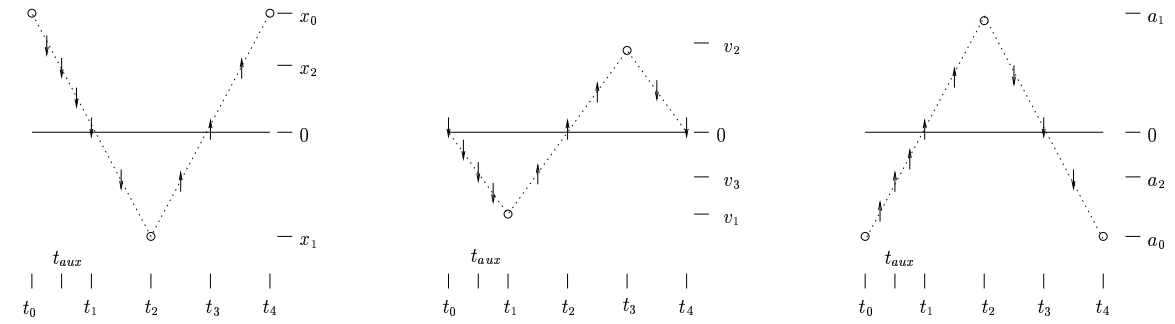


	x_0	x_1	v_1	v_2	a_0
range	$[8.3, 8.6]$	$[-8.6, -8.3]$	$[-3.04, -2.3]$	$[2.3, 3.04]$	$[-1.08, -0.638]$

	a_1	t_1	t_2	t_3	t_4
range	$[0.638, 1.08]$	$[2.73, \infty]$	$[5.46, \infty]$	$[8.19, \infty]$	$[10.9, \infty]$

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 [182].

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. The insertion of a new state at $t_{aux} = 1.36$, in the gap between t_0 and t_1 (figure 15), leads to an improvement of the bounds on the value the time landmarks. For example, the interval for t_1 is refined from $[2.73, \infty]$ to $[3.44, 14.4]$, as shown in figure 16. The interval bounds for the landmarks of the position, velocity, and acceleration of the mass remain unchanged in the example, though. The location of gaps and the interpolation of states are repeated until sufficiently precise results are obtained or no further refinements occur.



	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	$[3.44, 14.4]$	$[6.17, \infty]$	$[8.90, \infty]$	$[11.6, \infty]$

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 [182].

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 [114]. 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 [132]. 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 [182]. These programs have 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 [182, 183, 185]. 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 at a 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 eighties, 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 dynamical 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 up 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.

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 dynamical 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 dynamical 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 importants 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 dynamical systems theory. 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 dynamical systems. This framework would provide a common conceptual basis for different methods, each tailored to a particular class of dynamical systems, while being flexible enough to apply to qualitative as well as (partially) quantitative models. The development of this synthetic framework might profit from work on the analysis of hybrid systems and control theory, where ideas similar in spirit to qualitative simulation have emerged (*e.g.*, [3, 6, 7, 9, 127, 128, 177]).

A synthetic computational view on the qualitative analysis of dynamical systems should establish a solid basis for achieving further upscaling, required for most real-life applications in science and engineering. Shults and Kuipers [168] have started to explore one possible direction, consisting of the combination of qualitative simulation and techniques for *model checking* [13, 39]. 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 earlier ideas in the same line [32, 33, 116], 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 dynamical 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.*, [36, 38, 93, 95, 109, 135, 150, 151, 193, 194, 202, 207]), many issues remain to be explored.

Making predictions on the qualitative behavior of dynamical 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 internal structure of an experimental system from its observed behavior. Future methods for the qualitative analysis of dynamical systems must therefore be integrated with other reasoning methods focussing on such tasks as model building, model testing, model discrimination, and model revision. Ultimately, this may results in versatile computer environments for the analysis of dynamical systems, like the computer-supported discovery environments envisioned in [49] and the environment for nonlinear system identification explored in [28, 29, 30]. 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.

Acknowledgments. The author would like to thank Grégory Batt, Olivier Bernard, Philippe Dague, Jean-Luc Gouzé, Michel Page, Violaine Pillet, Louise Travé-Massuyès, and Ivayla Vatcheva for comments on draft versions of this report and other contributions. This paper is the English translation of

a book chapter appearing in L. Travé-Massuyès, P. Dague (eds), *Modèles et raisonnements qualitatifs*, Hermès, Paris, 269-329, 2003.

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Éditeur
INRIA - Domaine de Voluceau - Rocquencourt, BP 105 - 78153 Le Chesnay Cedex (France)
http://www.inria.fr
ISSN 0249-6399