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Mathematical Foundations of Qualitative Reasoning

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■ We examine different formalisms for modeling qualitatively physical systems and their associated inferential processes that allow us to derive qualitative predictions from the models. We highlight the mathematical aspects of these processes along with their potential and limitations. The article then bridges to quantitative modeling, highlighting the benefits of qualitative reasoning–based approaches in the framework of system identification, and discusses open research issues.

Modeling Physical Systems Qualitatively

The need to represent physical systems by models is common to all scientific and engineering domains. However, the modeling process encounters difficulties from both ends: A model must adapt to the knowledge available and the task it is built for. The possible limitations of traditional numeric methods with respect to these problems mean qualitative models can be a good alternative: (1) qualitative models cope with uncertain and incomplete knowledge, (2) a qualitative model output equals an infinity of numeric runs that are obtained at once in compact form, (3) the qualitative predictions provide the relevant qualitative distinctions in the system's behavior, and (4) the modeling primitives allow for a more intuitive interpretation.

A system's evolution can be tackled in discrete terms by defining states and events that trigger transitions between states. This point of view is generally the adopted one when continuous dynamics of behavior are not relevant. The originality of qualitative reasoning is to provide an intermediate level between discrete event and continuous models in which the state space is discretized into a number of finite states, and transitions between those states obey continuity constraints (Dague and MQ&D 1995; Hayes 1985; Travé-Massuyès, Dague, and Guerrin 1997).

Let us illustrate these ideas with the well-known pressure regulator (without friction) example (figure 1).

In figure 1, Q is the fluid flow through the pipe; P_i and P_o are the input and output pressure, respectively; V represents the opening or closing speed of the valve; and F the force that acts on the piston. If the domains of the variables are abstracted into a finite number of values; for example, if we only retain their signs, the possible behaviors of the pressure regulator are all captured by the following finite-state automaton, so-called *envisionment in qualitative reasoning* (de Kleer and Brown 1984) (figure 2).

Every state in figure 2 corresponds to the indicated variables' qualitative values, and the arrows represent the transitions between states. Circled states are instantaneous states, whereas squared states have a positive duration. Starting from an initial state, the possible system's (qualitative) behaviors are obtained as a sequence of chronologically ordered states from the different paths in the automaton. For example, the sequence [4, 5, 4, 5, 1, 2] represents a behavior in which F first oscillates between 0 and positive value (with V negative) and then becomes negative while V becomes 0.

Domain abstraction, which abstracts the real domain value of variables into a finite number of ordered symbols, is at the core of qualitative reasoning. Domain abstraction is complemented by functional abstraction, which allows one to state incompletely known functional relationships between quantities. For example, one might want to say that the flow

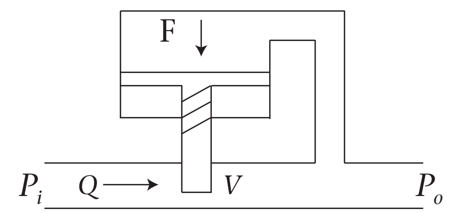

Figure 1. The Pressure Regulator.

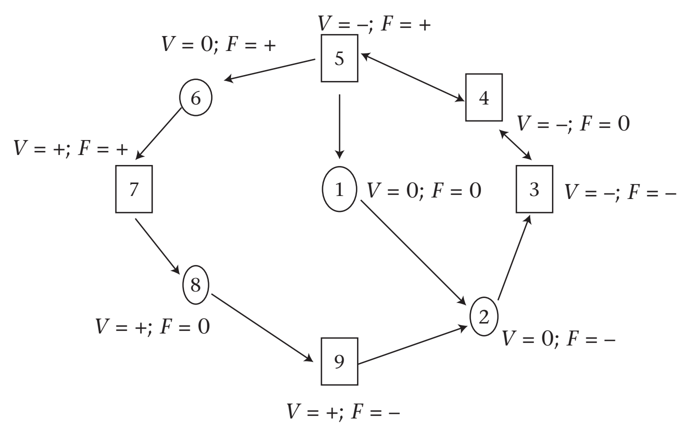

Figure 2. The Pressure Regulator Envisionment.

Figure 3. Landmarks for the Temperature of Water.

through a valve increases with the pressure difference, without specifying the particular function. Knowing some of their properties, such as monotonicity, is often sufficient to constrain the behavior of the variables. Domain and functional abstractions are associated with inferential processes, which perform on the quantities consistently with their numeric counterpart. They allow us to derive qualitative predictions of the system's state and perform simulation when the system is dynamic. We highlight the mathematical aspects of these processes along with their potential and limitations, with particular emphasis on qualitative simulation.

The section entitled Domain Abstraction and the Computation of Qualitative States and the section entitled Qualitative Simulation are concerned with the following questions, respectively: How can we compute the qualitative states of a system at a given time point? This question is answered by dealing with static models (traditionally represented by algebraic equations), for which resolution techniques have been proposed within different qualitative formalisms. How can we deal with temporal evolution and dynamics? This question puts the focus on dynamic models (traditionally represented by ordinary differential equations [ODEs]), for which behavior prediction calls for qualitative simulation techniques.

The last part of the article shows that some limitations of qualitative reasoning (Struss 1988) might be reduced significantly by the integration of such methods with either further knowledge on the mathematical properties of the specific system at study or partial quantitative knowledge or more sophisticated mathematics, borrowed, for example, from system theory. The article also highlights the need for qualitative reasoning–based approaches in the framework of quantitative modeling to perform quantitative system identification soundly and efficiently. Finally, the article concludes by discussing some open research issues.

Domain Abstraction and the Computation of Qualitative States

The central idea of qualitative reasoning is domain abstraction: It abstracts the value domain of continuous variables, which is generally the real line, into a finite number of ordered symbols representing qualitative values that make real behavioral distinctions. Domain abstraction is performed by identifying for each variable a set of distinguished points called *landmarks,* noted l_i, which partition the real line $\Re$.

Landmarks can be either numeric or symbolic because only their ordinal relationship is relevant. The qualitative value of a variable is either a landmark or an open interval between two adjacent landmarks. The finite, totally ordered set of all the possible qualitative values of a variable is called its *quantity space*. The quantity space can contain the landmarks $-\infty$, 0, and $+\infty$. For example, a natural set of landmarks for the temperature of water is given in figure 3.

It is obviously desirable that the mapping Q from real numbers to a finite quantity space verifies some properties. Real operators, *op,* for example, arithmetic operators, are qualitatively abstracted into operators *Q-op*. For example, if *op* is a binary operator, *Q-op* is usually defined as *a Q-op b* = {Q(*x op y*) | Q(*x*) = *a* and Q(*y*) = *b*}. More generally, a set *C* of real-valued constraints involving several operators can similarly be abstracted into a set of qualitative constraints *Q*(*C*). Let us note *Sol*(*C*), the set of all real solutions of a set of real-valued constraints *C,* and *Q-Sol*(*Q-C*), the set of all qualitative solutions of a set of qualitative constraints *Q-C*. Then we define the two following properties:

First, *Q* is said to be *sound* iff *Q*(*Sol*(*C*)) ⊆ *Q-Sol*(*Q*(*C*)) for any *C,* which is also equivalent to $\cup_{C|Q(C) = Q\text{-}C} Q(Sol(C)) \subseteq Q\text{-}Sol(Q\text{-}C)$ for any *Q-C*. It means that qualitative solutions of qualitative abstracted constraints capture the abstractions of all real solutions of real constraints, but some qualitative solutions can be spurious; that is, they do not correspond to any real solution of any real constraints compatible with the qualitative constraints.

Second, *Q* is said to be *complete* iff $Q\text{-}Sol(Q\text{-}C) \subseteq \cup_{C|Q(C) = Q\text{-}C} Q(Sol(C))$ for any *Q*-C, which means that each qualitative solution of a set of qualitative constraints is the abstraction of a real solution of a set of real constraints compatible with the qualitative constraints, but some real solutions might not be captured.

Ideally, we want *Q* to be sound and complete, but the next sections show that such property is generally not achievable.

Different domain abstractions capture different ways of reasoning qualitatively used by humans. In particular, the different intervals of a partition of $\mathcal{R}$ can be identified as orders of magnitude. The signs partition is a particular case, which was extensively used by economists (Ritschard 1983), then by the qualitative reasoning community (de Kleer and Brown 1984), to formalize reasoning about tendencies. In the following subsections, we present the mathematical structures and focus on the mathematical soundness of the formalisms.

Reasoning about Signs

Signs are useful for reasoning about the direction of change of variables describing a physical system: +, –, and 0 are used when the variable increases, decreases, and does not change, respectively. The problem is manipulating these signs to derive the direction of change of unknown variables or, in other words, computing the (signed) qualitative state of a system.

Consider a resistor, as in figure 4, and Ohm's law, which represents its physical behavior:

$$U = RI \quad (1)$$

where *R* is the resistance value, *U* is the voltage, and *I* the current. A simple analysis shows that if we know that *U* increases and that *R* remains steady, then *I* must also increase. To capture the various qualitative relations of this kind implied by equation 1, we write a *confluence* (de Kleer and Brown 1984), that is, a constraint on the signs of the directions of change of variables:

$$\partial U \approx \partial R + \partial I \quad (2)$$

The idea is to implement the well-known combinations of signs, such as (+) + (+) = (+), which is possible in the proper mathematical framework provided by sign algebra.

Let us consider the set *S* = {+, 0, –, ?}, in which the element ? is interpreted as *undetermined sign,* or *ambiguity*, and let us define the addition and multiplication of signs, as in figure 5. The element ? is important to guarantee that addition is a closed operator, for example, (+) + (–) is defined as ?. Whereas the relation = denotes the standard equality, ≈ is defined on *S* as follows:

For any *a* and *b* belonging to *S, a* ≈ *b* iff *a* = *b* or *a* = ? or *b* = ?.

≈ is called *qualitative equality* and can be interpreted as sign compatibility.

The algebraic properties of sign algebra have extensively been studied (Dormoy 1988; Piera and Missier 1989; Travé and Dormoy 1988). Some basic algebraic properties are as follows:

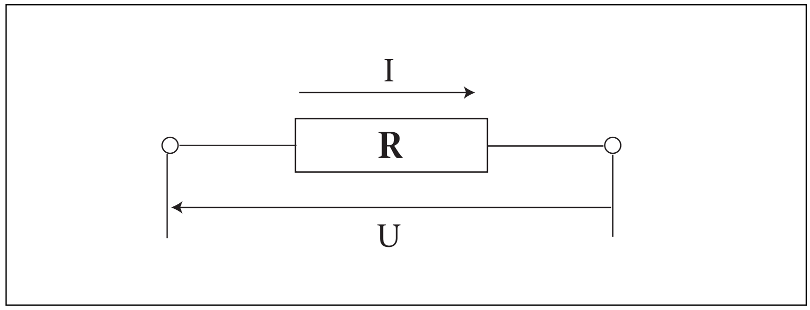

Figure 4. A Resistor.

+	0	+	-	?
0	0	+	-	?
+	+	+	?	?
-	-	?	-	?
?	?	?	?	?

*	0	+	-	?
0	0	0	0	0
+	0	+	-	?
-	0	-	+	?
?	0	?	?	?

Figure 5. Addition and Multiplication of Signs.

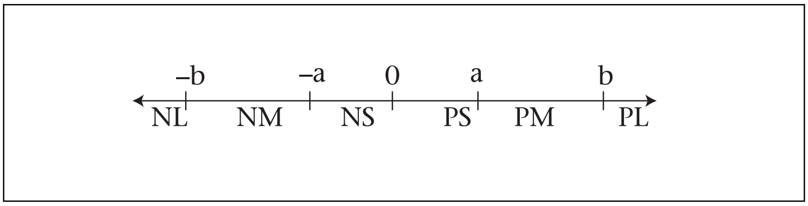

Figure 6. The Absolute Order-of-Magnitude (3) Model.

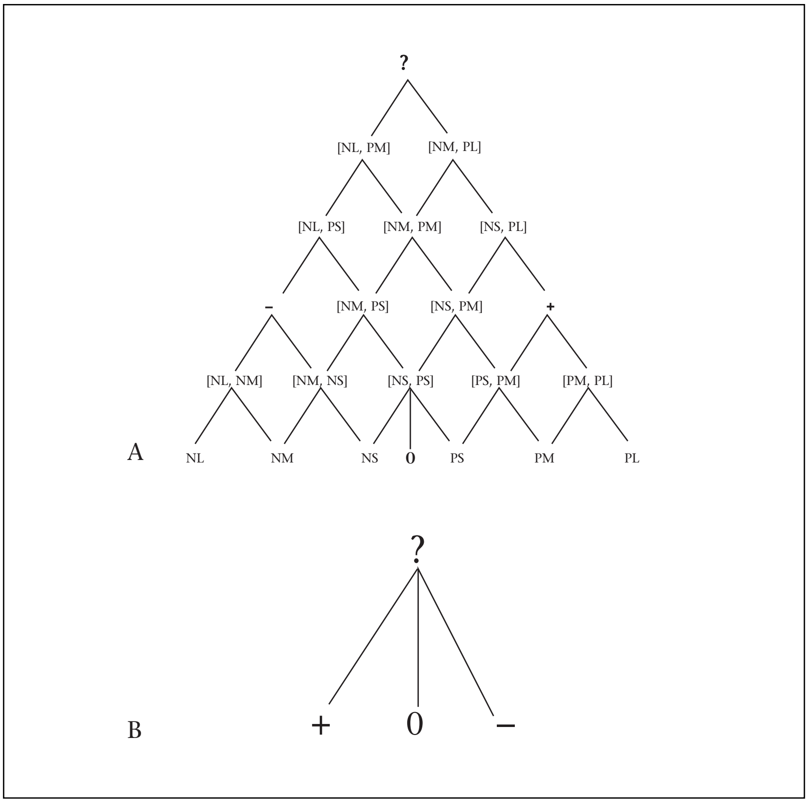

Figure 7. Absolute Order-of Magnitude Models Semilattice Structures.
A. Semilattice structure of (S, ≤). B. Semilattice structure of the sign model.

Quasi-transitivity of qualitative equality: If $a \approx b$ and $b \approx c$ and $b \neq ?$, then $a \approx c$.

Compatibility of addition and qualitative equality: $a + b \approx c$ is equivalent to $a \approx c - b$.

Qualitative resolution rule: Let $x, y, z, a,$ and b be qualitative quantities such that $x + y \approx a$ and $-x + z \approx b$. If x is different from ?, then $y + z \approx a + b$.

Coming back to our confluence (equation 2) and assuming that $\partial U = +$ and $\partial R = 0$, then equation 2 becomes $(+) \approx (0) + \partial I$, and it is easy to deduce that $\partial I \approx (+)$, which is the correct answer.

The simplistic example of the resistor can be generalized to much more complex systems, composed of many components. The whole system qualitative model is then obtained by assembling the components' confluences, resulting in a set of confluences. The property that $x^i = x$ or $-x$ for $x \in S$ means that we generally have to deal with qualitative equations that are linear. Such a set of confluences can be written in matrix form as $A\mathbf{X} \approx \mathbf{B}$, where A is a matrix, $\mathbf{X}$ the vector of variables (variations), and $\mathbf{B}$ the (constant) right-hand–side vector and is referred to as a *qualitative linear system* (QLS).

Mathematical properties of QLSs have been studied extensively (Travé and Dormoy 1988), and interesting notions such as qualitative rank and hard components have been defined, in relation to the problem of solving QLSs to compute the qualitative state of a system (Travé and Kaszkurewicz 1986; Travé-Massuyès, Dague, and Guerrin 1997). An important result is that unlike other more sophisticated qualitative algebras (cf. section entitled Absolute Orders of Magnitude), the results of processing signs are not only sound but also complete for QLSs (Travé-Massuyés, Dague, and Guerrin 1997).

Reasoning about Orders of Magnitude

Reasoning about orders of magnitude is a very natural way to reason qualitatively. Two types of reasoning about orders of magnitude—(1) absolute and (2) relative—have recently been identified (Trave´-Massuyès et al. 2002).

Absolute Orders of Magnitude

Absolute order-of-magnitude (AOM) *models* subsume and generalize the sign model. They allow one to characterize quantities with better distinctions than just signs. A common AOM model constructs S by partitioning the real line into seven classes corresponding to the labels: (1) negative large (NL), (2) negative medium (NM), (3) negative small (NS), (4) zero (0), (5) positive small (PS), (6) positive medium (PM), and (7) positive Large (PL) (cf. figure 6).

The AOM models rely on a partition of $\mathcal{R}$, which defines the quantity space S_1 based on a set of real landmarks including 0. S_1 generates the complete universe of description S of the AOM model as follows: $S = S_1 \cup \{[X, Y] \mid X, Y \in S_1 - \{0\}$ and $X < Y\}$, where $X < Y$ means that $\forall x \in X, \forall y \in Y, x < y$ in the sense of inferiority in $\mathcal{R}$, and the label $[X, Y]$ is defined as the smallest interval of the real line, with respect to the inclusion, that contains X and Y. If we now consider in S the order relationship induced by the inclusion, that is, for any pair $x, y \in S$, $x \leq y$ iff $x \subset y$, we obtain a semilattice structure, as shown in figure 7a, built up from the most precise to the least precise level. The sign model can be constructed in the same way from the sign partition, as shown in figure 7b.

Qualitative equality can now be formalized in a general way (generalizing sign compatibility), conveying the idea of possibility of being equal, that is, possibility that the items coincide at a higher precision level:

$x, y \in S$, $x \approx y$ iff there exists $z \in S$ such that $z \leq x$ and $z \leq y$.

Let us now define two internal operators in S, a q-sum $\oplus$ and a q-product $\otimes$, which are consistent with the real sum and product. It has been shown (Piera and Travé-Massuyès 1989; Piera, Sanchez, and Travé-Massuyès 1991; Travé-Massuyès, Piera, and Missier 1989) that $\oplus$ and $\otimes$ are compatible with $\approx$, are both Q-associative and Q-commutative,[2] and are such that $\otimes$ is distributive with respect to $\oplus$. Then, $(S, \oplus, \otimes, \approx)$ is defined as a *Q-algebra* (qualitative algebra of orders of magnitude).

For a given number of qualitative labels, the partition of $\mathcal{R}$ is not unique because it is dependent on the landmarks' numeric values. Hence, it is difficult to define symbolic operations by tables, and we must use the concept of qualitative function associated to a real function, which generalizes qualitative operators. Interesting properties referring to the reversibility of a qualitative relationship and the existence of a qualitative inverse are shown in Travé-Massuyès, Piera, and Missier (1989). The operators $\oplus$ and $\otimes$, also noted + and × when not ambiguous, are Q-reversible: $(A + B \approx C) \Leftrightarrow (B \approx C - A)$.[3] Hence in particular, $(A \approx B) \Leftrightarrow (B - A \approx 0)$; this equivalence is only true because 0 is an element of S. Similarly, if A is not qualitatively equal to 0, we have $(A \times B \approx C) \Leftrightarrow (B \approx C \times (1/A))$. If, however, $A \approx 0$ but $A \neq 0$, $1/A$ exists and equals ?; hence, the equivalence is still true even if it results in $B \approx$?.

The qualitative negation $[-A]$ (associated to real negation) can also be considered. It satisfies that for all $A \in S$, $[-A] = -A$ iff the partition is symmetric, in which case $[-A]$ is the qualitative opposite of A. However, as pointed out in Struss (1988), some severe limitations exist because of the lack of strict associativity and distributivity. For example, the result of a sequence of qualitative operations is not independent of the order in which the operations are performed. The different results are, however, always qualitatively equal, which actually means that the minimality of the solution is not guaranteed; in other words, the solution is sound but incomplete. Incompleteness is one of the origins of spurious behaviors in qualitative simulation, as is presented in the section entitled Qualitative Simulation.

Relative Orders of Magnitude

Another way to view orders of magnitude is to establish comparative relations between quantities, which is typically the way physicists and engineers proceed, by considering two quantities as negligible, comparable, or close. A typical example is the way a transistor is explained to students, as having the base current negligible with respect to the emitter current, which is, in turn, close to the collector current.

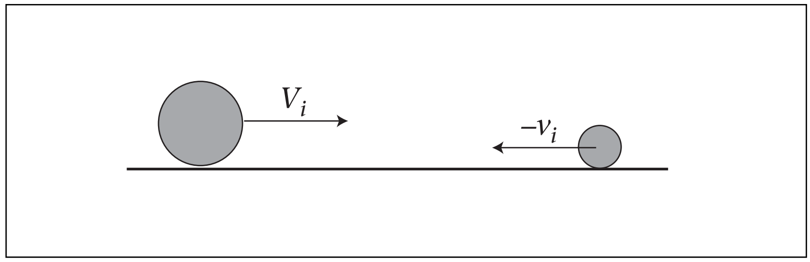

Figure 8. Example of Two Masses.

Relative order-of-magnitude (ROM) relations can be defined as binary relations, which boil down to a difference of values or a quotient of values belonging to an absolute partition. The first type is based on relations invariant by translation, whereas the second type is based on relations invariant by *homothety*, that is, by proportional transformation. Because they are closer to human intuition, all the ROM models proposed in the literature are based on binary relations r_i invariant by homothety; that is, $A\ r_i\ B$ only depends on the quotient A/B. Their axiomatization is described by a set of rules.

The first ROM model FOG (Raiman 1991) was based on three relations—(1) negligible with respect to (Ne), (2) close to (Vo), and (3) comparable to (Co, in the sense of "the same sign and order of magnitude as")—and included 32 inference rules that were proven to be true when giving the relations an interpretation in the field of real numbers of nonstandard analysis (NSA) (Robinson 1966), which roughly speaking is obtained from $\mathcal{R}$ by adding infinitely small and infinitely large numbers.

Reasoning with FOG can be illustrated through a simple example of mechanics (Raiman 1991): the impact of two masses of different weights, M and m, coming from opposite directions with close velocities V_i and v_i (cf. figure 8).

The two laws of momentum and energy conservation express that both $MV + mv$ and $MV^2 + mv^2$ remain the same before and after the impact. Based on only the signs, it is impossible to predict the directions of the masses after the impact. FOG makes it possible to use the assumptions m Ne M and V_i Vo $- v_i$ to correctly predict that the larger mass keeps the same direction, and the smaller one changes direction. Furthermore, one can deduce that the velocity of the larger mass after impact remains close to that before impact, and the velocity of the smaller one after impact becomes close to three times that before impact.

The ROM models that were developed later improved FOG not only in the necessary aspect of a rigorous formalization but also in the permitting of the incorporation of quantitative information and the control of the inference process to obtain valid results in the real world.

The formal model ROM(K) (Dague 1993b) proposed to add the relation Di standing for *distant from*. The four binary relations Ne, Vo, Co, and Di are defined by means of 15 axioms, which provide about 45 inference rules. ROM(K) has a nice symmetrical property and the ability to express gradual changes from one order of magnitude to another thanks to the existence of overlapping regions when interpreted in NSA.

It was then shown (Dague 1993a) how to transpose ROM(K) to $\mathcal{R}$ with a guarantee of soundness, resulting in the system ROM($\mathcal{R}$). ROM($\mathcal{R}$) permits the incorporation of quantitative information and obtains sound results while it maintains the semantics of the inference paths in terms of the four symbolic relations of ROM(K). ROM($\mathcal{R}$) relations, negligibility at order k (N_k), proximity at order k (P_k) and distance at order k (D_k) are defined in $\mathcal{R}$, parameterized by a positive real k. For example, given two real numbers x and y, then x is defined to be negligible at order k or k-negligible with respect to y, $x \; N_k \; y$, if $|x| \leq k \; |y|$.

The previously defined relations are matched to ROM(K) relations using two parameters k_1 and k_2 in the following way: Vo $\Leftrightarrow P_{k1}$, Co $\Leftrightarrow P_{1-k2}$, Ne $\Leftrightarrow N_{k1}$, Di $\Leftrightarrow D_{k2}$. A first group of ROM(K) axioms is satisfied for any k_1 and k_2. A second group requires the following constraint: $0 < k_1 \leq k_2 \leq 1/2$. The remaining axioms cannot be satisfied in $\mathcal{R}$. For these remaining axioms, Dague (1993a) proposes to calculate the order-of-magnitude precision loss of the conclusion in the worst case. Note that ROM($\mathcal{R}$) subsumes the O(M) model proposed earlier (Mavrovouniotis and Stephanopoulos 1988), which corresponds to the case $k_1 = k_2$.

ROM models consistent with $\mathcal{R}$ can be viewed as AOM models with respect to the quotients of quantities. The two degrees of freedom of ROM($\mathcal{R}$), that is, the parameters k_1 and k_2, determine the landmarks of the partition. For example, we have x Ne y if and only if x/y belongs to $[-k_1, k_1]$. Recently, Travé-Massuyès et al. (2002) bridged the ROM($\mathcal{R}$) and AOM models, examining under which conditions these models are fully consistent. Absolute qualitative labels of two quantities can be interpreted in terms of the corresponding relative relation(s), and conversely.

The results produced by a strict interpretation of ROM models grounded in $\mathcal{R}$ generally differ from what humans produce. A heuristic interpretation was even proposed for O(M), borrowing some rules not interpretable in $\mathcal{R}$ from FOG. Hence, the conflicting conclusion that strict $\mathcal{R}$-based interpretations, although providing sound results, do not match human ROM reasoning, but heuristic interpretations are not intellectually satisfying because they are not sound!

Other Models

Pushing orders of magnitude to their limits leads one to consider dominant parameters as the only parameters, and humans often adopt the analysis performed under these assumptions, which is known as *exaggeration reasoning:* Missier (1994) utilizes infinitesimals to represent the order of growth of a logarithmic-like function and utilizes them to perform asymptotic analysis; Weld (1990) uses exaggeration in conjunction with differential qualitative analysis techniques; Neitzke and Neumann (1994) use comparative analysis for simulation; and Williams and Raiman (1994) uses caricatural reasoning for decompositional modeling.

At the other end, reasoning about intervals, that is, about ranges of values, is frequently used in qualitative reasoning. The intervals formalism provides more flexibility than quantity space–based models, but the fact that intervals are not mapped onto qualitative labels makes their semantics weaker. A whole subfield of AI is devoted to this topic, known as numeric constraint-satisfaction problems (CSPs), which use consistency techniques based on interval arithmetic (Lhomme 1993).

Qualitative Simulation

Most physical systems exhibit dynamics that cannot be ignored. Then, dynamic models, traditionally represented by ODEs, are required. The question of dealing with temporal evolution and dynamics within a qualitative framework is answered by qualitative simulation.

From a historical perspective, there are three main approaches to reasoning about dynamic systems: (1) the *component-centered approach* of ENVISION by de Kleer and Brown (1984), (2) the *process-centered approach* of QPT by Forbus (1984), and (3) the *constraint-centered approach* of QSIM by Kuipers (1994, 1986). A flavor of the ENVISION approach was given in the section entitled Reasoning about Signs. It is based on confluences and adopts a quasi-static point of

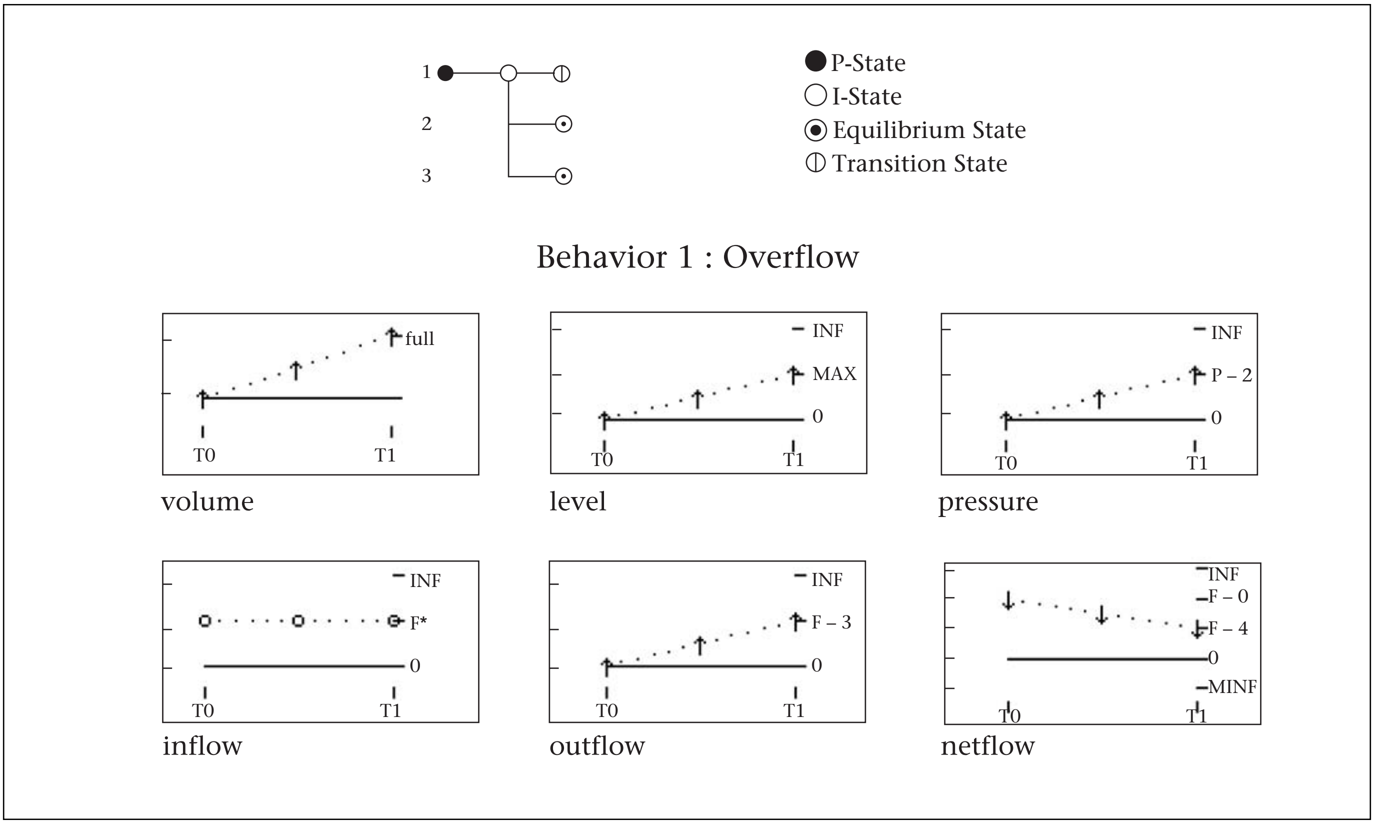

Figure 9. Bathtub Behavior Tree and Variable Plots for Behavior 1 (Bathtub Overflow).

view. QPT is grounded on two fundamental concepts: (1) *individual views,* which represent objects or sets of objects viewed from a particular perspective, and (2) *processes,* which represent active changes taking place (Forbus 1984). QSIM ignores the model-building task and focuses on qualitative simulation. A QSIM model is indeed simply given by a set of *qualitative differential equations* (QDEs), which are defined as an abstraction of ODEs.

All three approaches have been extremely influential on qualitative reasoning. Because QSIM shows a strong relationship with numeric simulation and allows for the integration of mathematical results related to ODEs, it has become the reference in terms of qualitative simulation over the years.

Time Representation

The first question to be answered about time is whether it should be qualitatively abstracted like other variable values. However, the answer depends on the task.

If the objective is to track the behavior of a system along time, based on observations delivered by sensors at given sampled time points, it is natural to consider these numeric time points as landmarks on the time axis. Determining the qualitative state can be performed at each time slice independently by checking the qualitative model against the observations for consistency. This so-called state-based approach (Struss 1997) is like dealing with a succession of static models. For a variable x, no relationship is expressed between dx/dt and x.

Most efficiently, some mathematical properties about transitions between time points, such as continuity or differentiability along time, can be used to constrain the behavior of the variables. For example, let's assume $x = a$ at time point t and also $x = a$ at time point t', $t' > t$. Then, if x is continuously differentiable, dx/dt necessarily equals 0 at one (at least) time point between t and t'.

However, using continuity and differentiability properties is often insufficient, and it is necessary to take advantage of the relationship between a variable and its derivative. Both have values in a finite quantity space consisting of landmarks and the intervals between landmarks. A linear interpolation is generally used, which leads to a constraint between $x(t)$, $dx/dt(t)$ and $x(t + 1)$. Because uncertainty on the variable gives rise to much higher uncertainty on its derivative, in most of the applications,

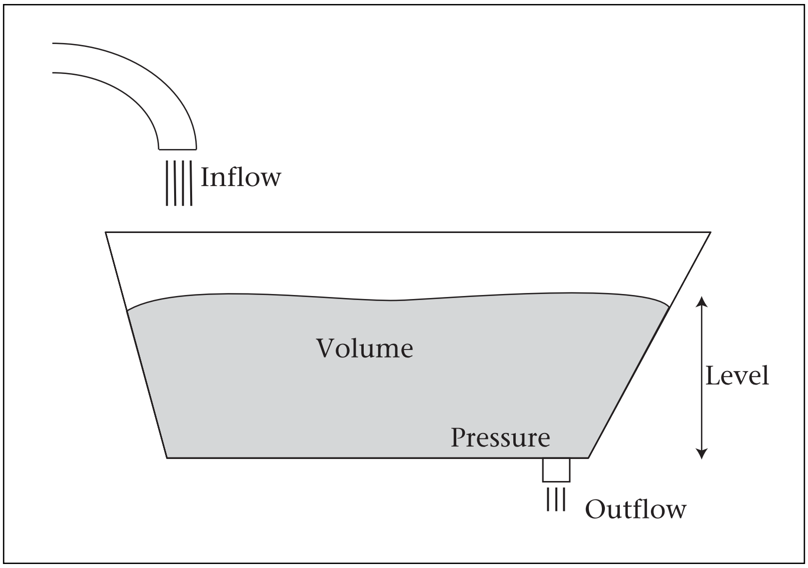

Figure 10. The Bathtub.

P1	$<l_j$, std>	→	$<l_j$, std>
P2	$<l_j$, std>	→	$<(l_j, l_{j+1})$, inc>
P3	$<l_j$, std>	→	$<(l_{j-1}, l_j)$, dec>
I1	$<(l_j, l_{j+1})$, inc>	→	$<l_{j+1}$, std>
I2	$<(l_j, l_{j+1})$, inc>	→	$<l_{j+1}$, inc>
I3	$<(l_j, l_{j+1})$, inc>	→	$<(l_j, l_{j+1})$, inc>
I4	$<(l_j, l_{j+1})$, inc>	→	$<(l_j, l_{j+1})$, std>

Table 1. Example of QSIM P-Transitions and I-Transitions.

the quantity space used for the derivatives is signs; that is, the direction of change of *x* is decreasing, steady, or increasing.

Continuity and differentiability assumptions can be expressed, such as in QSIM, in the form of transition tables for pairs $<x, dx/dt>$. Translation tables are obtained from the intermediate value and the mean-value theorems. *Time points* are defined as the instants at which the qualitative state of the system changes; that is, at least one variable or derivative reaches or leaves a landmark of its quantity space, as illustrated in figure 9, on the variable plots of the bathtub simulation. Hence, transitions apply either from one time point to the time interval starting at this time point (*P*-transitions) or from one time interval to its ending time point (*I*-transitions). Thus, time consists of a series of alternating points and open intervals between the points. The time points are not mapped onto physical time; they are just symbolic instants on which transitions occur, as in discrete-event models. The transition tables capture the constraints for a one-step prediction. They can be iteratively applied over several steps, achieving qualitative simulation.

Given l_{j-1}, l_j, and l_{j+1}, three adjacent landmarks in some variable quantity space, an example of QSIM P-transitions and I-transitions starting from the same state is given in table 1.

A consequence of this time representation is that when two transitions are possible, for example, *x* reaching landmark *a* and *y* reaching landmark *b,* very often the qualitative model does not constrain the ordering of these two events, which gives rise to temporal branching on whether one event occurs strictly before the other (and which one), or they occur simultaneously.

Paradoxically, qualitative time representation formalisms, such as the popular Allen (1983) algebra based on 13 primitive qualitative relations between two time intervals (such as before, after, beginning, ending, and during), do not fit within the qualitative simulation framework. The same is true for qualitative spatial models (Cohn and Hazarika 2001), which form a separate set of approaches.

Functional Abstraction through Qualitative Constraints

Very often, the functional relationship existing among a set of variables is abstracted through the use of relations instead of functions used in Domain Abstraction and the Computation of Qualitative States. For example, addition over the signs was defined as a function +: $S \times S \rightarrow S$ in Reasoning about Signs but can be considered as a relation $S^* \times S^* \times S^* \rightarrow$ {true, false}, where $S^* = S \backslash \{?\}$. By doing so, uncertainty propagation is lower.

Abstraction through relations can be generalized to several types of qualitative constraints, which restrict the set of possible values of the variables. Constraint-satisfaction techniques can then be used to check consistency. To illustrate this issue, let's take QSIM. For representing the behavior of a system, QSIM uses three kinds of qualitative constraints: (1) arithmetic, (2) differential, and (3) functional.

Arithmetic: ADD(x, y, z) for $z = x + y$, MULT(x, y, z) for $z = x. y$, MINUS(x, y) for $x = -y$.

Differential: DERIV(x, y) for $y = dx/dt$.

Functional: $M^+(x, y)$ ($M^-(x, y)$) for $y = f(x)$, and f is a strictly monotonically increasing (decreasing) function of x; that is, $y = f(x)$ with f differentiable and $f' > 0$ ($f' < 0$).

Nonmonotonic and multivariate qualitative constraints can also be defined (Kuipers 1986). In the bathtub example provided in the next subsection, the relationships between pressure and level and between level and volume are specified as M^+, and the system's dynamics comes from the constraint between volume and netflow, which is differential.

Constraints can be made more specific by means of *corresponding values,* which are tuples of landmarks from variables appearing in the constraint. For example, a correspondence <l_1, l_2> for $M^+(x, y)$, where l_1 and l_2 are landmarks, means that x is l_1 when y is l_2. In the bathtub example, the M^+ constraint between volume and level has two corresponding values (0 0) and (full max). The proper choice of landmarks has a critical impact on the qualitative simulation results. Irrelevant landmarks can indeed cause undesired branching.

A QDE generally has a limited domain of validity. First, the quantity space of some variables can be restricted, as in the bathtub example for which 0 is the lower bound of the quantity spaces of the volume, level, pressure, outflow, and inflow variables. Second, different operating regions can be specified. Discontinuities can be modeled by means of operating region transitions, triggered on detection of a variable taking some qualitative value. The bathtub model specifies one such transition, indicating that as soon as the qualitative value of volume is <full, inc>, then the bathtub overflows. Hence, simulation within this region stops or is resumed in another operating region, corresponding to another QDE.

```
(define-QDE Bathtub
   (quantity-spaces
         (volume (0 full inf))
         (level (0 max inf))
         (pressure (0 inf))
         (outflow (0 inf))
         (inflow (0 f* inf))
         (netflow (minf 0 inf)))
   (constraints
         ((M+ volume level) (0 0) (full max))
         ((M+ level pressure) (0 0) (inf inf))
         ((M+ pressure outflow) (0 0) (inf inf))
         ((ADD netflow outflow inflow))
         ((d/dt volume netflow))
         ((constant inflow))))
   (transitions
         ((volume (full inc)) -> tub-overflows)))
```

Figure 11. QSIM *Model of the Bathtub.*

The QSIM Simulation of the Bathtub Example

Let's consider the bathtub in figure 10. The bathtub is filled with a constant inflow and has a drain, which evacuates an outflow. The initial state is an empty bathtub. The other variables are the volume and the level of water and the bottom pressure. We assume that we do not know the exact values for inflow and outflow or the physical dimensions of the bathtub, but we want to predict the behavior of the bathtub.

The QSIM model of the bathtub is given in figure 11. Qualitative simulation starts from the initial state and repeatedly generates all possible successor states. Because in general the successor state cannot be determined uniquely, QSIM branches at every possibility. This potential for a branching sequence of events is an important difference between qualitative and numeric simulation. QSIM thus builds a tree of states: *Nodes* are system states, and *edges* are transitions between states; a *behavior* is a path from the root of the tree to a leaf. The behavior tree for the bathtub given in figure 9 shows three possible behaviors: The level stabilizes (1) under max, (2) at max, or (3) overflows.

A leaf of the tree of states is obtained when a state is a *no-change state*; that is, its successor would be identical, would be a *cycle* (that is, is identical to one of its predecessors), or is quiescent (that is, all the directions of change are steady, which means that the state is an equilibrium state or contains at least one variable taking on an infinite value).

Behavior Abstraction

Qualitative models are a proper abstraction of real-valued models in the sense that they represent a class of real-valued models. The structural abstraction theorem of QSIM proves that each ODE can be abstracted into a QDE such that any continuously differentiable function that is a solution of the ODE also satisfies the QDE. Conversely, a QDE is an abstraction of a whole class of ODEs.

The behavior abstraction theorem states, illustrated by figure 12,[4] that the behavior of a set of continuously differentiable functions $F = \{f_1,...,f_n\}$ defined over a bounded interval $[t_0, t_n]$ can be abstracted uniquely into a qualitative behavior $QB(F, [t_0, t_n])$ given by a sequence of qualitative states. However in general, the same qualitative behavior corresponds to a whole class of continuously differentiable functions.

Properties of Qualitative Simulation

From the results in the previous subsection, it can be shown that given a QDE, qualitative simulation generates all the qualitative behaviors corresponding to the solutions of any ODE in the abstracted class. However, generated be-

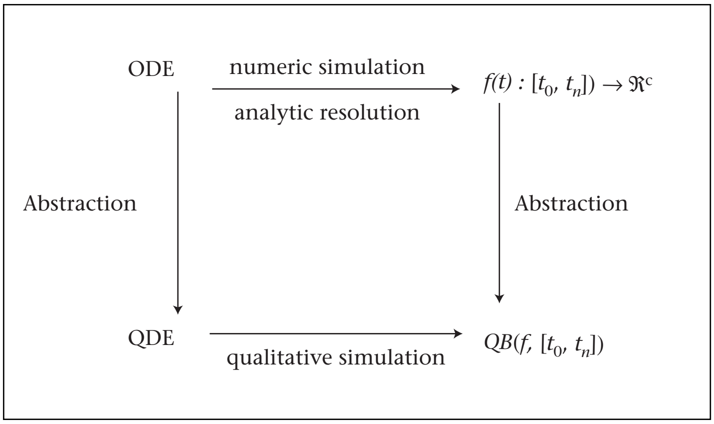

Figure 12. Behavior Qualitative Abstraction.

haviors eventually include so-called spurious qualitative behaviors. Hence, qualitative simulation is sound but incomplete.

Spurious behaviors are an undesirable feature, and many solutions have been provided, depending on the cause: spurious qualitative states (Struss 1988), spurious state transitions (Kuipers et al. 1991), or spurious sequences of qualitative states (Fouché and Kuipers 1992; Lee and Kuipers 1993). However, in spite of the proposed solutions, qualitative simulation has recently been demonstrated inherently incomplete (Say and Akin 2002).

Another important problem is that the number of possible (nonspurious) behaviors can be enormous, causing the behavior trees to be intractable and difficult to interpret. Among the causes of this problem are occurrence branching, which is the result of incomplete specification of the functions leading to irrelevant qualitative distinctions, and chattering variables, which are totally unconstrained variables (Clancy and Kuipers 1997; Kuipers et al. 1991).

Toward Integrated Approaches: Combining Quantitative and Qualitative Knowledge

Qualitative simulation approaches, exemplified by QSIM, are trapped in the local nature of the algorithm and the specific formulation of a qualitative model in terms of constraints. Alternative approaches have been proposed. They have been shown powerful and can be viewed as contributions toward a unified modeling approach.

First is use more quantitative information, such as the semiquantitative simulation approach, including quantitative extensions of QSIM such as Q2 and Q3 (Berleant and Kuipers 1997; Kuipers 1994) that preserve the underlying qualitative semantics and interval model-based simulation (Armengol et al. 2000; Haber and Unbehauen 1990; Piera, Sanches, and Travé-Massuyès 1991; Raiman 1991). Second is take the benefit of results in the area of systems theory, such as the qualitative phase-space analysis approach (Bernard and Gouzé 2002; de Jong et al. 2003; Dordan 1992; Ross et al. 1999). Third is integrate qualitative reasoning with traditional engineering modeling approaches such as numeric simulation or system identification. The first point is exemplified by the self-explanatory simulation stream (Forbus 1984), and the third point is presented in more detail in the next section.

System Identification: The Need for Qualitative Reasoning–Based Approaches

System identification (Ljung 1987) aims at deriving a quantitative model of a dynamic system from observations of its output in response to input. System identification is crucial in science and technology because it allows us to get insights into a number of domains and perform a wide spectrum of tasks where quantitative information about the system dynamics is required. System identification is quite a complex process that basically involves the experimental data and a model space to search for the best model. The construction of the model space strictly depends on the available domain knowledge: When it is sufficient to represent the underlying physics of the processes involved (gray box system), the model space, generally ODEs, is derived by the proper combination of the physical laws; when knowledge of the internal system structure is incomplete, or no first principles are available (black box system), the model space is represented by opportune function classes, generally nonlinear, that approximate the functional relationship between system input and output. In both frameworks, system identification mainly occurs in two phases: (1) *structural identification,* or selection within the model space of the equation form, and (2) *parameter estimation,* evaluation of the numeric values of the equation unknown parameters from the observations.

Structural identification is a crucial and difficult step. In the gray case, an initial guess of candidate models is suggested by the qualitative properties of the observed behavior, but it is feasible only if the modeler's background includes thorough knowledge of both mathematics and the specific domain. In the black case, it concerns the choice of the appropriate function complexity; here, the major drawback regards the result accuracy: The built model

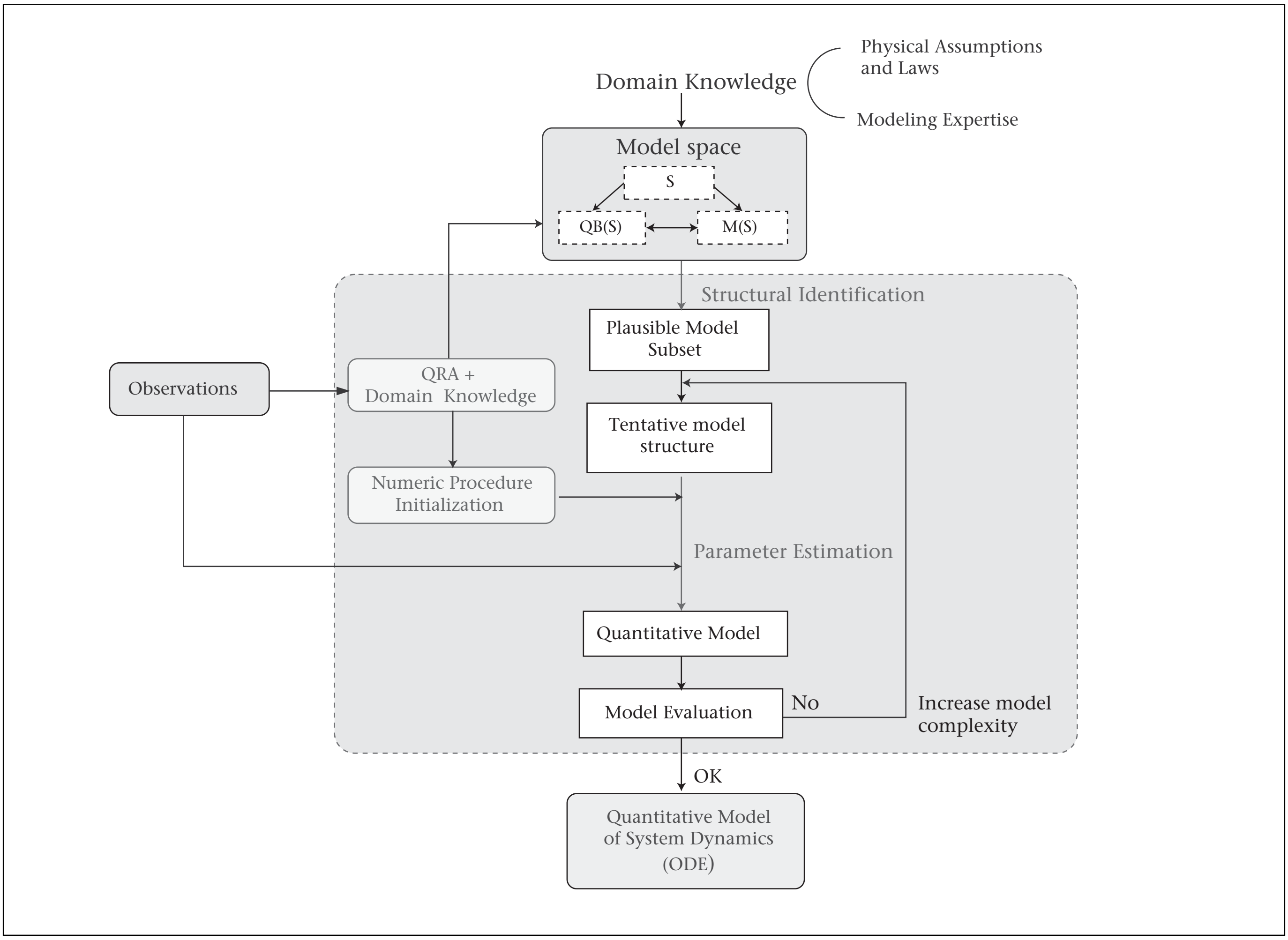

Figure 13. Gray Box Systems.

Qualitative reasoning–based system identification process. *S*: physical structure; *QB* and *M*: its qualitative behavior and mathematical model, respectively.

does reproduce the observations but does not capture the underlying physical reality, which can yield the inadequacy of model-predictive capability in many cases, for example, when the data sample is either small or noisy. In both contexts, the parameter-estimation problem can also be ill posed, and it might not converge to the true solution if a "good" guess of the parameter vector is not provided.

Qualitative reasoning techniques naturally complement both approaches: In one case, they allow us either to supply with the necessary knowledge or to emulate the expert's reasoning about structural identification; in the other, when the box is not completely black, which quite often occurs, they allow us to easily choose the proper equation complexity but, above all, to embed a priori knowledge with a significant gain in model robustness. To highlight the considerable advantages offered by qualitative reasoning–integrated approaches, we consider gray and black box systems, separately.

Gray Box Systems

RHEOLO (Capelo, Ironi, and Tentoni 1998), SQUID (Kay, Rinner, and Kuipers 2000), and PRET (Bradley, Easley, and Stolle 2001) are the most significant results of the application of qualitative reasoning methods to differential modeling. SQUID, based on QSIM semiquantitative extensions, only deals with the refinement of a single semiquantitative differential equation that represents the whole model space, whereas both RHEOLO and PRET deal with automated system identification and, in outline, follow the reasoning flow depicted in Figure 13. PRET is a general tool for linear and nonlinear system identification, and its performance depends on the knowledge it has about the target system at a given stage of the model-building process. On the contrary, RHEOLO is tailored to a specific domain, namely, the rheological behavior of *viscoelastic materials,* that is, materials whose behaviors result from a

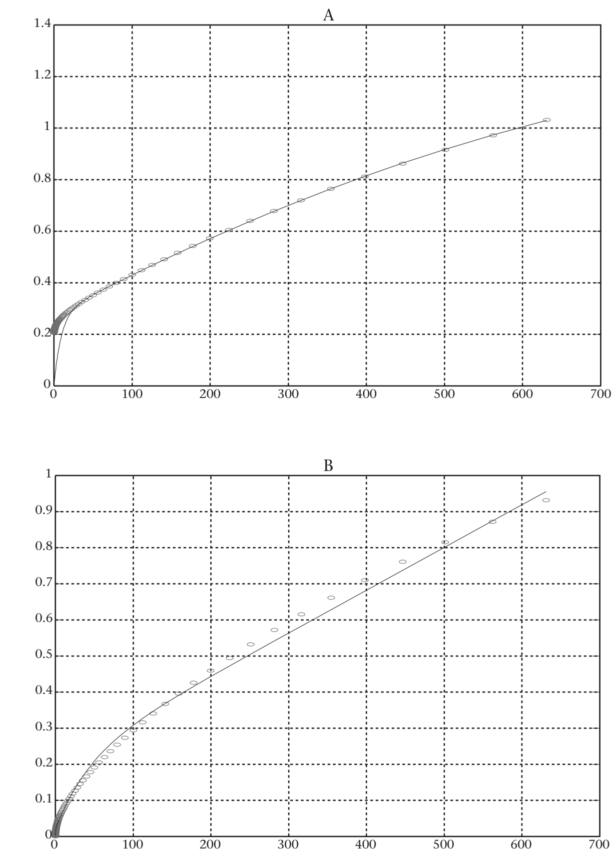

Figure 14. Weighted Least Squares Fitting of the Strain Response of Two Materials with Different Physical Properties.

The dots and the curve represent the time course of the data and the model prediction, respectively.

suitable combination of elastic and viscous responses.

Let us focus on RHEOLO to illustrate the great potential in terms of modeling soundness, computational costs, and actual applicability of qualitative reasoning integrated approaches. RHEOLO aims at the formulation of the most accurate ODE model that explains a set of observations obtained from standard tests on a material. Let us observe that in a quantitative context, the term *accuracy* can be misinterpreted as referring to numeric accuracy only. However, a model goes beyond a mere fitting: It must also capture all the physical features qualitatively expressed by the data. To exemplify this point, let us consider figure 14: The data sets are related to two materials that exhibit instantaneous elasticity, delayed elasticity, viscosity (figure 14a), and delayed elasticity and viscosity (figure 14b), respectively. However, at a pure numeric level, they are accurately modeled by an ODE with the same mathematical structure as the discontinuity in the data in figure 14a at $t = 0$, which does represent instantaneous elasticity, is smoothed by the numeric procedures. The identification of the appropriate mathematical structure precedes the quantitative refinement step and occurs on qualitative arguments only.

In the complex domain of viscoelasticity, the mathematical knowledge and skillfulness necessary for structural identification rarely belongs to researchers who, as designers of new materials, would benefit from models to assess the material properties. As a matter of fact, researchers mostly perform either (1) the material assessment experimentally, with high costs and poor informative content, or (2) a blind search over a possibly incomplete model space that might yield a model that fails to capture both the material complexity and all the material features (Capelo, Ironi, and Tentoni 1996).

The restriction to a well-defined domain largely compensates for the lack of generality. The specific domain knowledge has allowed for the development of ad hoc qualitative methods, and their integration with numeric and statistical ones has provided an efficient and sound solution to the problem of associating a real viscoelastic material with its constitutive law. In particular, thanks to these methods, a sound and complete simulation algorithm has ben designed, which has allowed us to associate each model of an ideal material in the model space with its qualitative behavior in response to standard experiments. On the basis of the qualitative responses, it has been possible to provide a small but significant contribution to the domain itself: the model space characterization and its partition into model classes featured by the same qualitative behavior. The model space M, automatically generated following an enumerative procedure and a component-connection paradigm in accordance with the domain knowledge, does exhaustively represent the viscoelastic material domain, to the extent of the underlying assumptions. Although the enumeration process has exponential complexity, the partition of the model space into qualitatively coherent classes has allowed us to achieve optimal linear, rather than exponential, computational costs.

Let us consider M, which consists of triples $(S, QB(S), M(S))$, where S is the material composite structure the ODE model $M(S)$ is built on and $QB(S)$ its simulated qualitative behavior.

Then, the subset of plausible structures is derived in a straightforward manner by matching the qualitative profiles of the data, obtained through qualitative response abstraction (QRA), against all the *QB*(*S*)s in M. QRA infers a qualitative description of the observed response by mapping geometric patterns extracted from the data plot into basic physical features. Qualitative simulation and QRA are fundamental to guaranteeing physical accuracy of the identified model because they characterize the relevant physical features of each model in the space and of the actual material dynamics, respectively.

Then, the best quantitative model is searched for in the candidate subset, hierarchically organized, through an optimization loop. Such a loop is initialized with the simplest parameterized model and proceeds with more and more complex structures until the optimal order of the model is found in accordance with a principle of parsimony. This loop nests the parameter estimation procedure, aimed at evaluating the optimal parameter vector that completely identifies the model of the material. Such a procedure uses a numeric differentiation scheme, which must suitably be selected to calculate a sound numeric solution. Moreover, to ensure convergence, "good" guesses must be provided for the parameters and the initial values of the differential numeric scheme. Both numeric problems benefit from QRA (Capelo, Ironi, and Tentoni 1996): The abstracted qualitative data profile suggests both the choice of an ODE solver capable of dealing with stiff solutions and the shape of a function to be used to calculate the initial parameter guess through a collocation method of the current ODE on the experimental grid.

RHEOLO issues a new challenge in the practical study of materials. Because of the underlying modeling assumptions, it finds its proper application to polymers, such as those used in pharmaceutics, cosmetics, and the food industry. Its applicative potential is shown by Rossi et al. (1999) and Ironi and Tentoni (2003): It allowed for the model-based assessment of the mucoadhesion property of a class of pharmaceutical polymers, a candidate for use as a drug carrier in a drug delivery system.

Black-Box Systems

The reconstruction of a relationship *f* between the input-output variables from observations is a difficult problem that has been studied intensively (Haber and Unbehauen 1990). Approximation schemes, directly applicable and widely used, are neural networks, multi-variate splines, and fuzzy systems (Wang 1994). Although successfully applied to many systems, they fail when the data set is inadequate (Bellazzi et al. 2001). Moreover, the resulting model *f* does not capture any structural knowledge.

Qualitative reasoning can effectively help to solve these problems in a great deal of situations: Physical system knowledge is often available even if insufficient to formulate a quantitative model, and it could conveniently be embedded into black-box methods. FS-QM (Bellazzi, Guglielmann, and Ironi 2000) integrates fuzzy systems with qualitative models (figure 15). It solves the crucial problem of the construction of a meaningful fuzzy rule base. The mathematical interpretation of such a rule base, automatically generated by encoding the state distinctions of the system dynamics inferred by the qualitative simulation of a QSIM model, defines both the complexity and the form of *f*. Then, the estimation of its parameter vector θ, initialized accordingly to prior information (θ_0), completes the system identification process.

The embodiment of physical knowledge into *f*, brought in by qualitative models, allows us to get efficient and robust results both in rich and poor data contexts, as demonstrated by applications of FS-QM to metabolic systems. More precisely, it has successfully been applied (1) to study the dynamics of the blood glucose level in diabetic patients in response to insulin therapy and meal ingestion (Bellazzi et al. 1998) and (2) to identify the dynamics of intracellular thiamine in the intestine tissue. Concerning the second system, neither the classical compartmental approach nor the input-output regression schemes provided acceptable results (Bellazzi et al. 2001).

Conclusion and Open Issues

This article highlights the mathematical foundations of formalisms proposed to mimic human qualitative reasoning along with potential and limitations. Qualitative inferences are shown to rely on solid theoretical ground, ensuring that qualitative models are a proper abstraction of real-valued models.

This article is not intended as a comprehensive overview of qualitative reasoning. Some important aspects have been omitted, such as causality, which is crucial when we want to explain the behavior of a system (de Kleer and Brown 1984; Iwasaki and Simon 1986). However, the presented concepts and tools show that qualitative representation offers a significant modeling methodology. However, it suffers limitations that can be imputed to the generality of the proposed approaches along with the

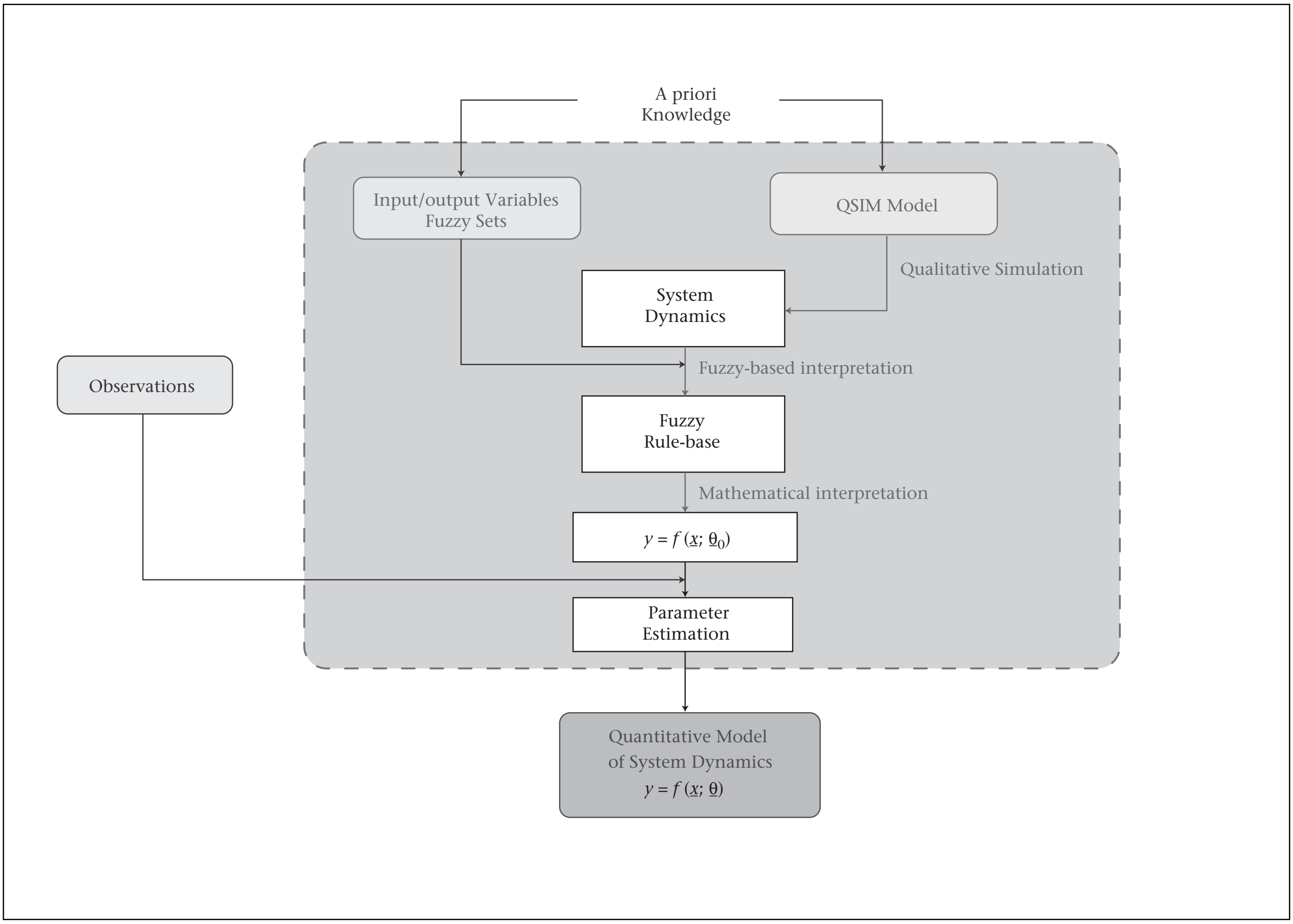

Figure 15. Black-Box Systems: Main Steps of FS-QM.

weakness of qualitative information. The first steps, illustrated in the article, toward the development of qualitative reasoning methods tailored to specific classes of problems, as well as their integration with numeric-statistical methods, have confirmed that unified modeling approaches can provide solutions that outperform either pure qualitative or pure quantitative approaches.

The automation of the modeling process is one of the open questions, in particular how to bridge the conceptual and higher abstraction models of qualitative reasoning to engineering models (Struss et al. 2002). Determining a set of relevant landmarks from the input-output of numeric quantitative models is a complex task. The landmarks are indeed conceptually defined as strong invariant points over the different operating regions of a system, which must be opposed to the local nature of numeric models.

Compositional modeling is also of great interest. For current practice in numeric modeling, the composition operation, resulting in an aggregate ODE (or constraint) model, is performed in the head of the modeler who knows the changes underlying model fragment composition. To be automated, this process calls for *influence resolution,* that is, the process of transforming a complete set of influences on each variable to constraints, so the resulting model will support simulation. Hence, it requires the concept of influence and the explicit representation of the phenomena occurring when assembling two fragments. Although qualitative reasoning has contributed to this topic, and qualitative process theory can be quoted in this respect (Falkenhainer and Forbus 1991; Forbus 1984), this issue remains open.

Notes

1. Liliana Ironi was particularly in charge of the section entitled System Identification: The Need for Qualitative Reasoning–Based Approaches, together with some editing of the entire article.

2. Same definitions as associative and commutative but replacing = by ≈.

3. Qualitative subtraction is defined as the qualitative function associated to real subtraction.

4. $\mathcal{R}^c = \mathcal{R} \cup \{-\infty, +\infty\}$.

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