Mathematical Foundations of Qualitative Reasoning

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ABSTRACT

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 paper then bridges to quantitative modeling, highlighting the benefits of QR-based approaches in the framework of system identification, and discusses open research issues.

1. Modeling physical systems qualitatively

The need to represent physical systems by models is common to all scientific and engineering domains. But the modeling process encounters difficulties from both ends: a model must adapt to the knowledge available and to the task it is built for. The possible limitations of traditional numeric methods with respect to these problems mean qualitative models may be a good alternative:

- qualitative models cope with uncertain and incomplete knowledge;
- a qualitative model output equals an infinity of numerical runs that are obtained at once in compact form;
- the qualitative predictions provide the relevant qualitative distinctions in the system's behavior;
- the modeling primitives allow for a more intuitive interpretation.

[1] Liliana Ironi has been more particularly in charge of section 4, together with some editing of the whole paper.

A system's evolution may be tackled in discrete terms, by defining states and events that trigger transitions between states. This is generally the adopted point of view when continuous dynamics of behavior are not relevant. The originality of QR 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 [26][13][55].

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

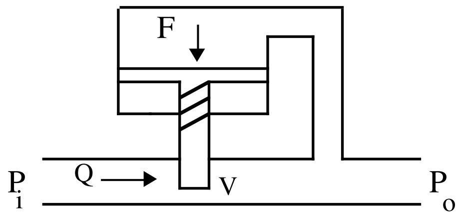

Figure 1 — *The pressure regulator*

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 QR [17].

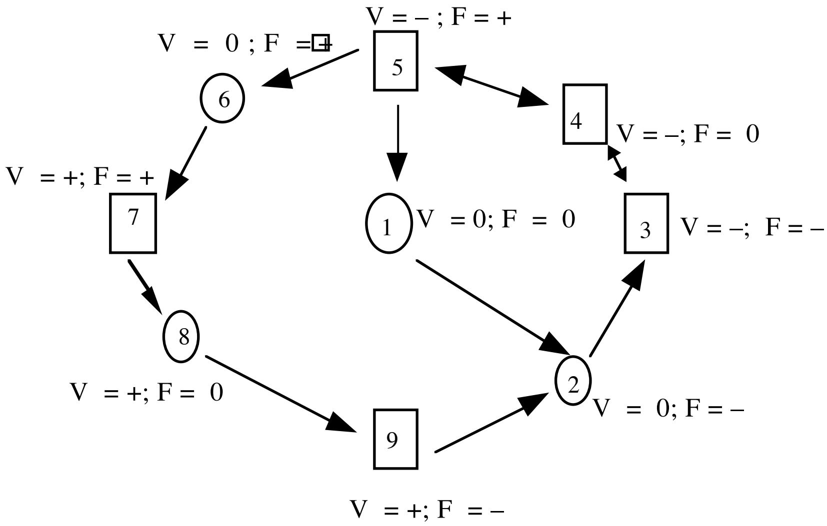

Figure 2 — *The pressure regulator envisionment*

Every state corresponds to the indicated variables qualitative values and the arrows represent the transitions betweens 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 instance, 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 QR. This is complemented by *functional abstraction,* which allows one to state incompletely known functional relationships between quantities. For instance, one might want to say that the flow 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. This is all 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 to 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.

Sections 2 and 3 of the paper are concerned with the questions:

- *How can we compute the qualitative states of a system at a given time point?* This comes back to dealing with static models (traditionally represented by algebraic equations), for which resolution techniques have been proposed for different qualitative formalisms.
- *How can we deal with temporal evolution and dynamics?* This puts the focus on dynamic models (traditionally represented by Ordinary Differential Equations (ODE's)), for which behavior prediction calls for *qualitative simulation* techniques.

The last part of the paper shows that some limitations of QR [52] may be significantly reduced 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 paper also highlights the need for QR-based approaches in the framework of quantitative modeling, to perform soundly and efficiently quantitative system identification. Finally, the paper concludes by discussing some open research issues.

2. Domain abstraction and the computation of qualitative states

The central idea of QR 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. This is performed by identifying for each variable a set of distinguished points called *landmarks*, noted l_i, which partition the real line .

Landmarks may be either numeric or symbolic as 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 may contain the landmarks –• , 0 and +• . For example, a natural set of landmarks for the temperature of water is given by:

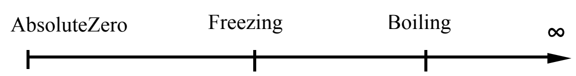

Figure 3 — *Landmarks for the temperature of water*

It is obviously desirable that the mapping *Q* from real numbers to a finite quantity space verifies some properties. Real operators, *op*, e.g. 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:

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

Ideally, we want Q to be sound and complete, but we will see that this is generally not achievable.

Different domain abstractions capture different ways of reasoning qualitatively used by humans. In particular, the different intervals of the partition can be identified as *orders-of-magnitude*. The signs partition is a particular case, which has been extensively used first by economists [45] then by the QR community [17] to formalize reasoning about tendencies. In the following sections, we present the mathematical structures, and focus on the mathematical soundness of the formalisms.

2.1 Reasoning about signs

Signs are very useful to reason 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 to manipulate these signs so as to derive the direction of change of unknown variables, or in other words to compute the (signed) qualitative state of a system.

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

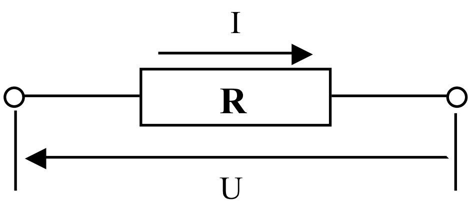

Figure 4 — *A resistor*

(eq. 1) $U=RI$

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* [17], that is a constraint on the signs of the directions of change of variables:

(eq. 2) $\partial U \approx \partial R + \partial I$

and the idea is to implement the well-known combinations of signs, such as '(+) + (+) = (+)'. This 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 Table 1. The element ? is important to guarantee that addition is a closed operator, e.g. (+) + (–) is defined as ?.

+	0	+	–	?
0	0	+	–	?
+	+	+	?	?
–	–	?	–	?
?	?	?	?	?

*	0	+	–	?
0	0	0	0	0
+	0	+	–	?
–	0	–	+	?
?	0	?	?	?

Table 1— *Addition and Multiplication of signs*

Whereas the relation = denotes the standard equality, ≈ is defined on *S* as follows:

For any a and b belonging to S,

$a \approx b$ *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 been extensively studied [19][53][57]. Some basic algebraic properties are:

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, 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 (eq. 2), and assuming that $\partial U=+$ and $\partial R=0$, then (eq. 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 $AX \approx B$, where *A* is a matrix, *X* the vector of variables (variations), and *B* the (constant) right-hand side vector, and is referred to as a *Qualitative Linear System* (QLS).

Mathematical properties of QLSs have been extensively studied [53], and interesting notions such as *qualitative rank* and *hard components* have been defined, in relation with the problem of solving QLSs to compute the qualitative state of the system [54][55]. An important result is that, unlike other more sophisticated qualitative algebras (cf. section 2.2.1) the results of processing signs are not only sound but also complete for QLSs [55].

2.2 Reasoning about orders-of-magnitude

2.2.1 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 7 classes corresponding to the labels: Negative Large (NL), Negative Medium (NM), Negative Small (NS), Zero (0), Positive Small (PS), Positive Medium (PM) and Positive Large (PL) (cf. figure 5).

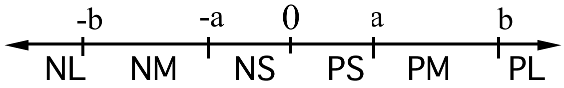

Figure 5 — *The AOM(3) model*

The AOM models rely on a partition of $\mathbb{R}$ 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:

$$S = S_1 \cup \{[X, Y] \mid X, Y \in S_1 - \{0\} \text{ and } X < Y\}$$

where $X < Y$ means that $\forall x \in X, \forall y \in Y, x < y$ in the sense of inferiority in $\mathbb{R}$, 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, i.e. for any pair $x, y \in S$, $x \leq y$ iff $x \subseteq y$, we obtain a semi-lattice structure as shown in Figure 6(a), 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 6(b).

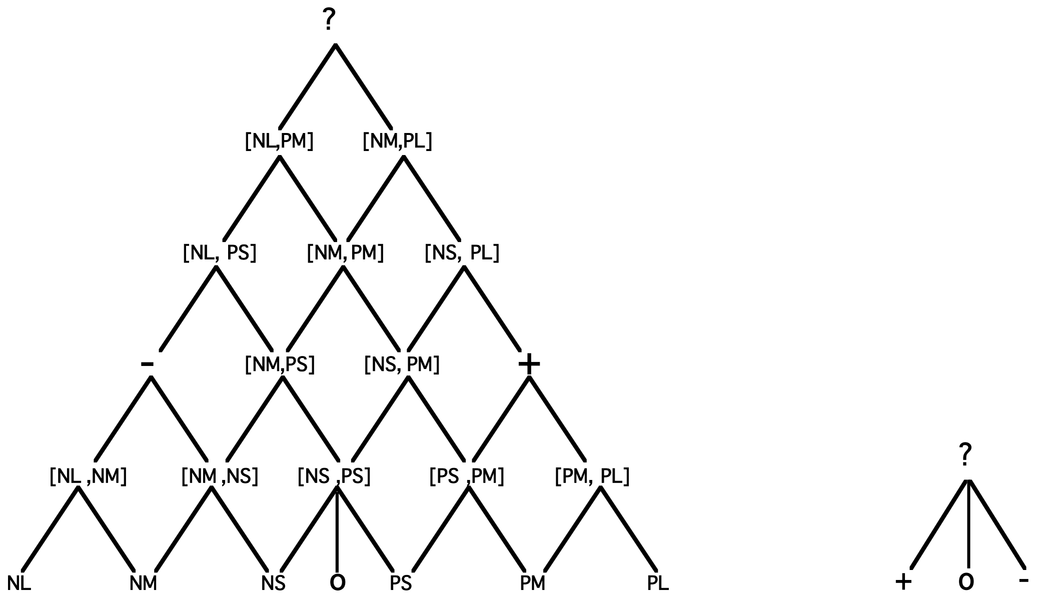

Figure 6 — (a) *Semi-lattice structure of (S,≤);* (b) *Semi-lattice structure of the sign model*

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

x, y □ *S, x* ≈ *y* iff there exists *z* □ *S* such that *z* □*x* and *z* □*y*.

Let us now define two internal operators in *S*, a q-sum ⊕ and a q-product , which are consistent with the real sum and product. It has been shown [40][41][57] that ⊕ and are compatible with ≈, are both Q-associative, Q-commutative[2], and are such that is distributive with respect to ⊕. Then, (S, ⊕, ,≈) is defined as a *Q-algebra (Qualitative algebra of orders of magnitude*).

For a given number of qualitative labels, the partition of is not unique, since dependent of the landmarks numerical values. It is hence 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 [57]. The operators ⊕ and , also noted + and □ when not ambiguous, are Q-reversible: *(A + B ≈ C)* □ *(B ≈ C – A)*[3]. Hence in particular: *(A ≈ B)* □ *(B – A ≈ 0)*, this equivalence being only true because 0 is an element of *S*. Similarly, if *A* is not qualitatively equal to 0, we have *(A* □*B ≈ C)* □ *(B ≈ C* □ *(1/A))*. If however *A ≈ 0* but *A ≠ 0, 1/A* exists and equals ?; hence the equivalence is still true even if it results in *B ≈ ?*.

The qualitative negation *[–A]* (associated to real negation) can also be considered. It satisfies that for all *A* □ *S*, *[–A] = –A* iff the partition is symmetric, in which case *[–A]* is the qualitative opposite of *A*. But, as pointed out in [52], some severe limitations exist due to the lack of strict associativity and distributivity. For instance, 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, or in other words that the solution is sound but incomplete. This is one of the origins of spurious behaviors in qualitative simulation, as will be presented in section 3.

2.2.2 Relative orders-of-magnitude

Another way to view orders-of-magnitude is by establishing comparative relations between quantities. This 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.

Relative orders-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. 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, i.e. $A\ r_i\ B$ only depends on the quotient *A/B*. Their axiomatization is described by a set of rules.

The first ROM model FOG [43] was based on three relations, *"negligible with respect to"* (Ne), *"close to"* (Vo) and *"comparable to"* (Co, in the sense of "the same sign and order of

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[2] Same definitions as associative and commutative, by replacing = by ≈.

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

magnitude as"), and included 32 inference rules which were proven to be true when giving the relations an interpretation in the field of real numbers of N.S.A. (Non Standard Analysis) [46], which roughly speaking is obtained from   by adding infinitely small and infinitely large numbers.

Reasoning with FOG can be illustrated through a simple example of mechanics [43]: the impact of two masses of very different weights, M and m, coming from opposite directions with close velocities V_i and v_i (cf. figure 7).

Figure 7 — *Example of two masses*

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. Considering 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 while 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 permitting 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) [15] proposed to add the relation Di standing for *"distant from"*. The four binary relations Ne, Vo, Co, 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 N.S.A.

It was then shown [14] how to transpose ROM(K) to   with a guarantee of soundness, resulting in the system ROM( ). ROM( ) permits the incorporation of quantitative information and obtains sound results while maintaining the semantics of the inference paths in terms of the four symbolic relations of ROM(K). ROM( ) relations, negligibility at order k (N_k), proximity at order k (P_k) and distance at order k (D_k), are defined in , parameterized by a positive real k. For instance, 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 above defined relations are matched to ROM(K) relations using two parameters k_1 and k_2 in the following way: Vo □ P_{k1}, Co □ P_{1-k2}, Ne □ N_{k1}, Di □ 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 . For those, [14] proposes to calculate the order-of-magnitude precision loss of the conclusion in the worst case. Note that ROM( ) subsumes the O(M) model proposed earlier [37], which corresponds to the case $k_1=k_2$.

ROM models consistent with   can be viewed as AOM models with respect to the quotients of quantities. The two degrees of freedom of ROM( ), i.e. the parameters k_1 and k_2, determine the landmarks of the partition. For instance, we have x Ne y if and only if x/y

belongs to $[-k_1, k_1]$. A recent piece of work [56] has bridged ROM( ) 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 generally differ from what humans produce. A heuristic interpretation was even proposed for O(M), borrowing some rules not interpretable in from FOG. This leads to the conflicting conclusion that strict based interpretations, although providing sound results, do not match human ROM reasoning but heuristic interpretations are not intellectually satisfying because they are not sound!

2.3 Other models

Pushing orders-of-magnitude at their limits leads one to consider dominant parameters as the only parameters and humans often adopt the analysis performed under these assumptions. This is known as *exaggeration reasoning*: in [38], infinitesimals represent the order-of-growth of a logarithmic-like function and are used to perform *asymptotic analysis*; in [59] exaggeration is used in conjunction with differential qualitative analysis techniques; in [39] comparative analysis is used for simulation; in [60] *caricatural reasoning* is used for decompositional modeling.

At the other end, *reasoning about intervals*, i.e. about ranges of values, is frequently used in QR. 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 sub-field of AI is devoted to this topic, known as *numeric CSP* (Constraint Satisfaction Problems), which use consistency techniques based on interval arithmetic [35].

3. Qualitative simulation

Most physical systems exhibit dynamics that cannot be ignored. Then, dynamic models, traditionally represented by Ordinary Differential Equations (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: the *component centered* approach of ENVISION by de Kleer and Brown [17]; the *process centered* approach of QPT by Forbus [21]; and the *constraint centered* approach of QSIM by Kuipers [30][31]. A flavor of the ENVISION approach has been given in section 2.1. It is based on confluences and adopts a quasi-static point of view. QPT is grounded on two fundamental concepts: *Individual Views*, which represent objects or sets of objects viewed from a particular perspective, and *Processes*, which represent active changes taking place [21]. 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 QR. As QSIM shows a strong relationship with numerical 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.

3.1 Time representation

The first question to be answered about time is whether it should be qualitatively abstracted, like other variable values, or not. But 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 numerical time points as landmarks on the time axis. Determining the qualitative state can be performed at each time slice independently, by checking for consistency the qualitative model against the observations. This so-called state-based approach [50] 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 *x=a* at time point *t'*, *t'>t*, as well. Then if *x* is continuously differentiable, *dx/dt* necessarily equals 0 at one (at least) time point between *t* and *t'*.

However, this 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 made up 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)*. As uncertainty on the variable gives rise to much higher uncertainty on its derivative, in most of the applications, the quantity space used for the derivatives is signs, i.e. the direction of change of *x* is decreasing, steady, or increasing.

Continuity and differentiability assumptions can be expressed, like in QSIM, in the form of transition tables for pairs $<x, dx/dt>$. These 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 10 on the variable plots of the bathtub simulation. Transitions hence 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*). Time consists thus 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:

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

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 algebra based on 13 primitive qualitative relations between two time intervals (such as before, after, beginning, ending, during, etc.) [1], do not fit within the qualitative simulation framework. The same is true for qualitative spatial models [12], which form a separate set of approaches.

3.2 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 section 2. For instance, addition over the signs was defined as a function +: $S \times S \rightarrow S$ in section 2.1, but can be considered as a relation: $S^* \times S^* \times S^* \rightarrow$ {true, false}, where $S^*=S \setminus \{?\}$. By doing so, uncertainty propagation is lower.

This 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*:

- *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, i.e. $y = f(x)$ with f differentiable and $f' > 0$ ($f' < 0$).

Non-monotonic and multivariate qualitative constraints can also be defined [31]. In the bathtub example provided in section 3.3, the relationships between `pressure` and `level` and between `level` and `volume` are specified as M+ and 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 critical impact on the qualitative simulation results. Irrelevant landmarks may indeed cause undesired branching.

A QDE has generally 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, 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 that region stops or is resumed in another operating region, corresponding to another QDE.

3.3 The QSIM simulation of the bathtub example

Let's consider the bathtub of figure 8. The bathtub is filled in 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`, neither the physical dimensions of the bathtub but we want to predict the behavior of the bathtub.

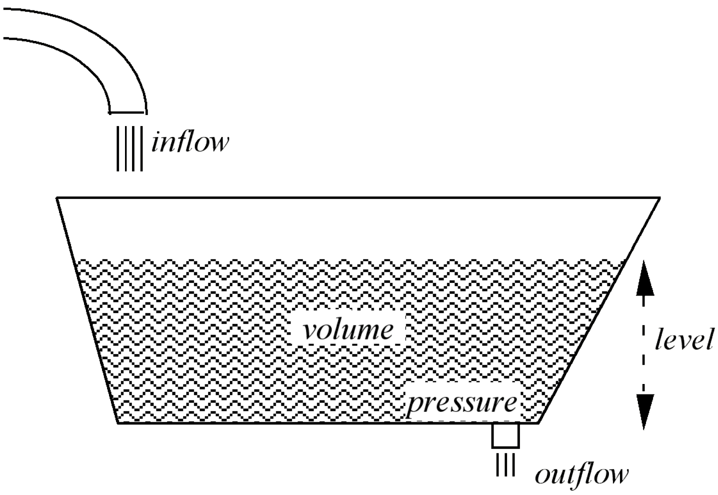

Figure 8 — *The bathtub*

```
(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 9 — *QSIM model of the bathtub*

The QSIM model of the bathtub is given in figure 9. Qualitative simulation starts from the initial state, and repeatedly generates all possible successor states. As in general the successor state cannot be determined uniquely, QSIM branches on every possibility. This potential for a branching sequence of events is an important difference between qualitative and numerical 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 10 shows three possible behaviors: the level stabilizes under `max`, at `max` or overflows.

A leaf of the tree of states is obtained when a state is a ‘no change’ state, i.e. its successor would be identical, or is a cycle, i.e. is identical to one of its predecessor or is quiescent, i.e. 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.

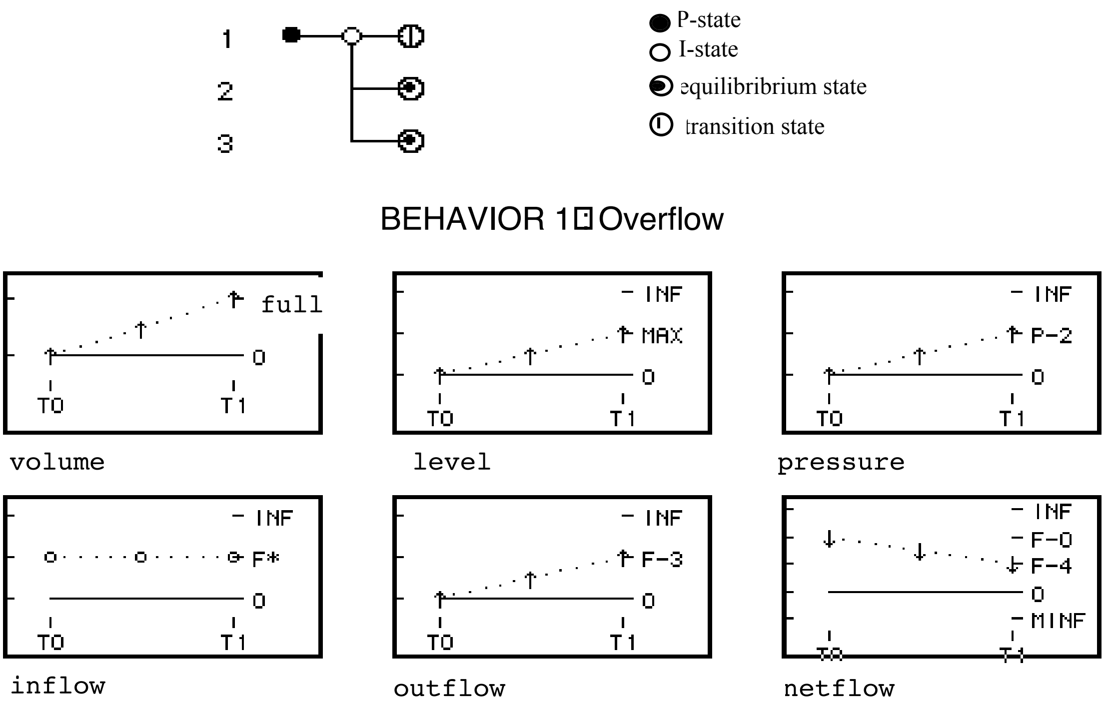

Figure 10 — *Bathtub behavior tree and variables plots for behavior 1 (bathtub overflow)*

3.4 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 11[4], that the behavior of a set of continuously differentiable functions $F=\{f_1,\ldots,f_n\}$ defined over a bounded interval $[t_0, t_n]$ can be uniquely abstracted into a qualitative behavior QB(F, $[t_0, t_n]$) given by a sequence of qualitative states. But in general, the same qualitative behavior corresponds to a whole class of continuously differentiable functions.

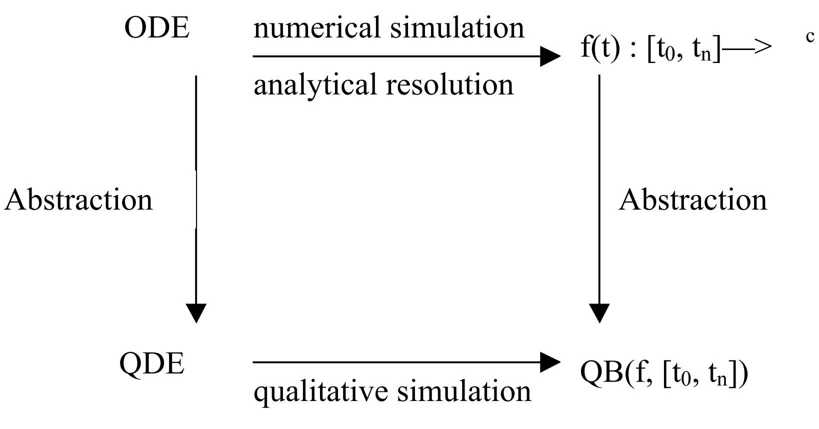

Figure 11 — *Behavior qualitative abstraction*

[4] $\Re^c = \Re \cup \{-\infty, +\infty\}$.

3.5 Properties of qualitative simulation

From the results in section 3.4, 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 behaviors eventually include so-called *spurious qualitative behaviors*. Qualitative simulation is hence *sound* but *incomplete.*

Spurious behaviors are an undesirable feature and many solutions have been provided, depending on the cause: spurious qualitative states [52], spurious state transitions [33], or spurious sequences of qualitative states [23] [34]. But in spite of the proposed solutions, qualitative simulation has been recently demonstrated inherently incomplete [49].

Another important problem is that the number of possible (non-spurious) behaviors may be enormous, causing the behavior trees to be intractable and difficult to interpret. Among the causes of this problem are *occurrence branching,* due to incomplete specification of the functions leading to irrelevant qualitative distinctions, and *chattering variables*, which are totally unconstrained variables [11][33].

3.6 Towards 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, of three types, have been proposed, which have been shown powerful and can be viewed as contributions towards a unified modeling approach:

- Use more quantitative information, like the semi-quantitative simulation approach including (1) quantitative extensions of QSIM like Q2 and Q3 [32][6] which preserve the underlying qualitative semantics; (2) interval model based simulation [2] [44][42][25].
- take benefit of results in the area of systems theory, like the qualitative phase space analysis approach [48][18][7][16].
- integrate QR with traditional engineering modeling approaches like numerical simulation or system identification. The first is exemplified by the self-explanatory simulation stream [22] and the latter is presented in more details in section 4.

4. System Identification: the need for QR-based approaches

System Identification (SI) [36] aims at deriving a *quantitative* model of a dynamic system from observations of its outputs in response to inputs. SI is crucial in science and technology as it allows us to get insights into a great deal of domains, and to perform a wide spectrum of tasks where quantitative information about the system dynamics is required. It is a quite complex process that basically involves the experimental data, and a model space where 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 ODE's, 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 inputs and output. In both frameworks, SI mainly occurs in two phases:

- *Structural identification*: selection within the model space of the equation form;
- *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 does reproduce the observations but does not capture the underlying physical reality. This may yield the inadequacy of model predictive capability in many cases, e.g. when the data sample is either small or noisy. In both contexts, the parameter estimation problem may also be ill posed, and it may not converge to the true solution if a "good" guess of the parameter vector is not provided.

QR 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 QR-integrated approaches, we consider gray and black box systems, separately.

4.1 Gray box systems

RHEOLO [10], SQUID [29], and PRET [8] are the most significant results of the application of QR methods to differential modeling. SQUID, based on QSIM semi-quantitative extensions, only deals with the refinement of a single *semi-quantitative differential equation* that represents the whole model space; whereas both RHEOLO and PRET deal with automated SI, and in outline follow the reasoning flow depicted in Figure 12. PRET is a general tool for linear and nonlinear SI, 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 suitable combination of elastic and viscous responses.

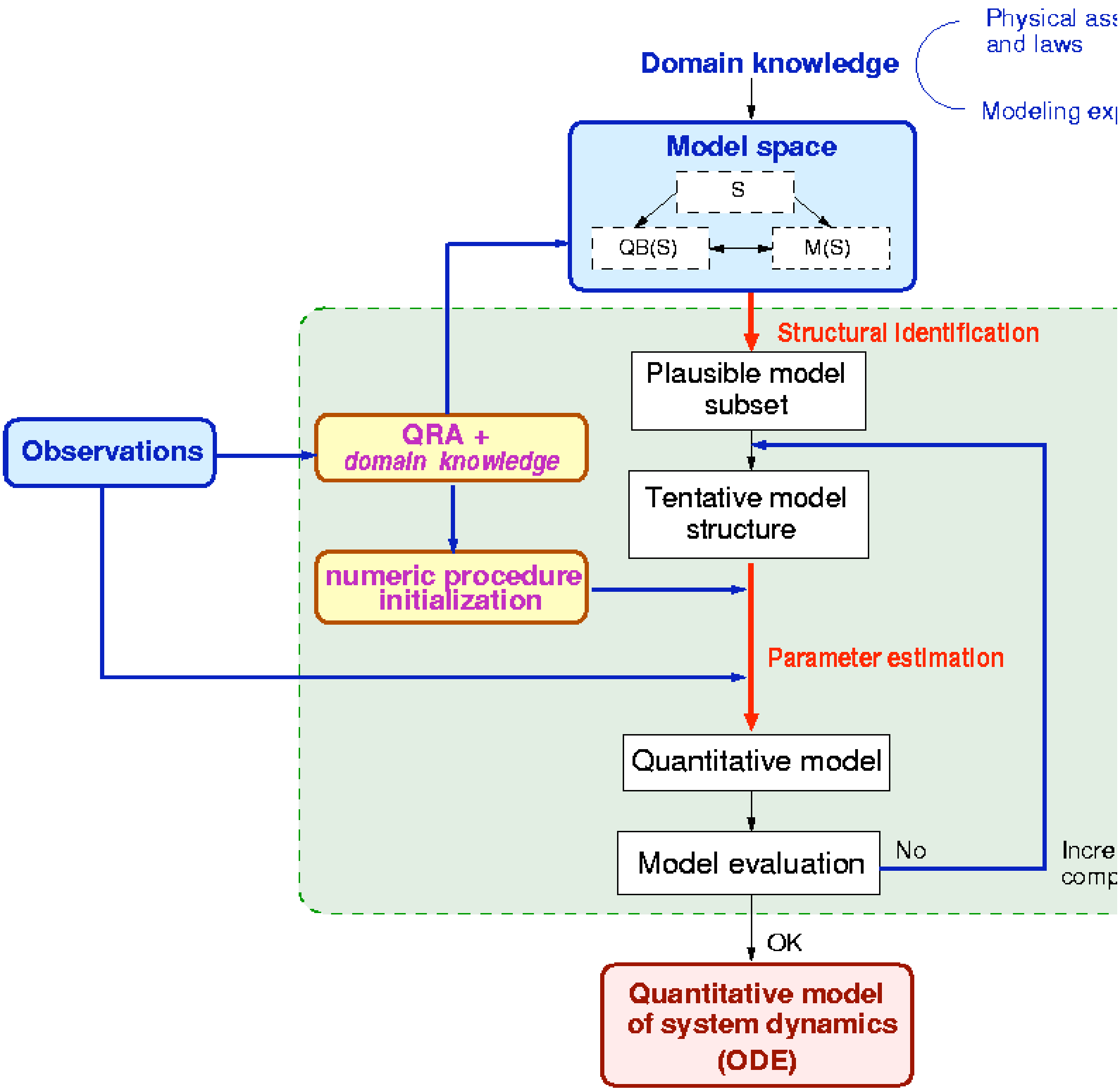

Figure 12 – *Gray box systems: QR-based system identification process. S: physical structure; QB and M: its qualitative behavior and mathematical model, respectively.*

Let us focus on RHEOLO to illustrate the great potential, in terms of modeling soundness, computational costs and actual applicability of QR-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" may be misinterpreted as referring to numerical accuracy only. But 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 13: the data sets are related to two materials which exhibit instantaneous elasticity, retarded elasticity, viscosity (Figure 13A), and retarded elasticity, viscosity (Figure 13B), respectively. But, at a pure numerical level they are accurately modeled by an ODE with the same mathematical structure as the discontinuity in the data in Figure 13A at $t = 0$, which does represent instantaneous elasticity, is smoothed by the numerical 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 (i) the material assessment experimentally, with high costs and poor informative content, or (ii) a blind search over a possibly incomplete model space that may yield a model that fails to capture both the material complexity and all the material features [9].

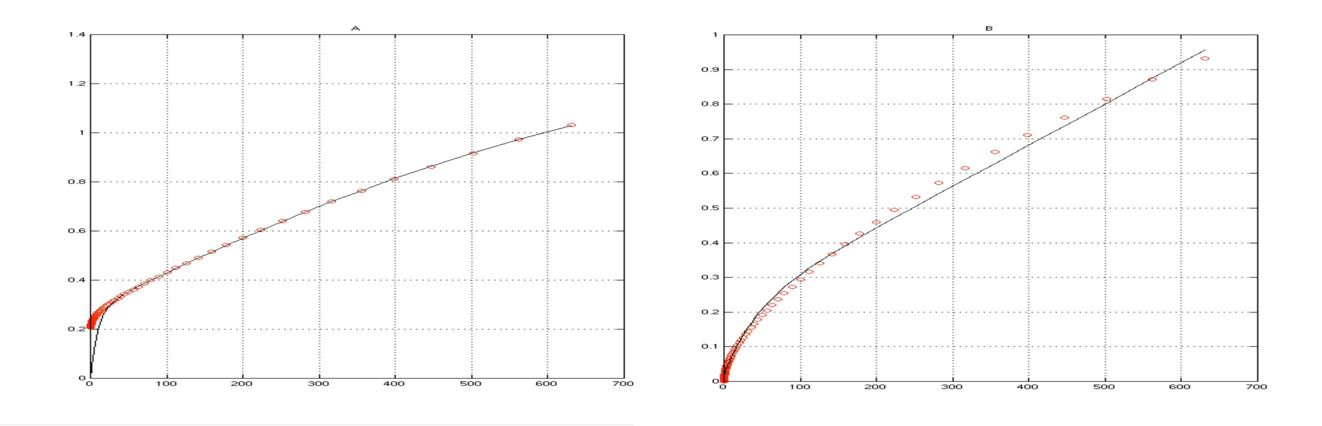

Figure 13 – *Weighted least squares fitting of the strain response of two materials with different physical properties. The dots and the curve represent the time course of the data and the model prediction, respectively.*

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 numerical 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 upon and *QB*(*S*) its simulated qualitative behavior. Then, the subset of plausible structures is straightforward derived: 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 guarantee *physical accuracy* of the identified model as 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 till 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 numerical differentiation scheme, which must suitably be selected to calculate a sound numerical solution. Moreover, to ensure convergence, "good" guesses must be provided for the parameters and the initial values of the differential numerical scheme. Both numerical problems benefit from QRA [9]: the abstracted qualitative data profile suggests both the choice of an ODE solver capable to deal 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. Due to the underlying modeling assumptions, it finds its proper application to polymers, such as those used in Pharmaceutics, Cosmetics, and Food Industry. Its applicative potential is shown in [47][27]: it allowed for the model-based assessment of the mucoadhesion property of a class of pharmaceutical polymers, candidate for use as a drug carrier in a drug delivery system.

4.2 Black box systems

The reconstruction of a relationship *f* between the input-output variables from observations is a difficult problem, intensively studied [24]. Approximation schemes, directly applicable and widely used, are neural networks, multi-variate splines, and fuzzy systems [58]. Although successfully applied to many systems, they fail when the data set is inadequate [4]. Moreover, the resulting model *f* does not capture any structural knowledge.

QR may effectively help to solve the problems above in a great deal of situations: physical system knowledge is very often available even if insufficient to formulate a quantitative model, and it could be conveniently embedded into black box methods. FS-QM [3] integrates fuzzy systems with qualitative models (Figure 14). It solves the crucial problem of the construction of a meaningful fuzzy rule-base. The mathematical interpretation of such 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 SI 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 (i) to study the dynamics of the blood glucose level in diabetic patients in response to insulin therapy and meal ingestion [5], and (ii) to identify the dynamics of intracellular thiamine in the intestine tissue. Concerning the latter system, both the classical compartmental approach and input-output regression schemes did not provide acceptable results [4].

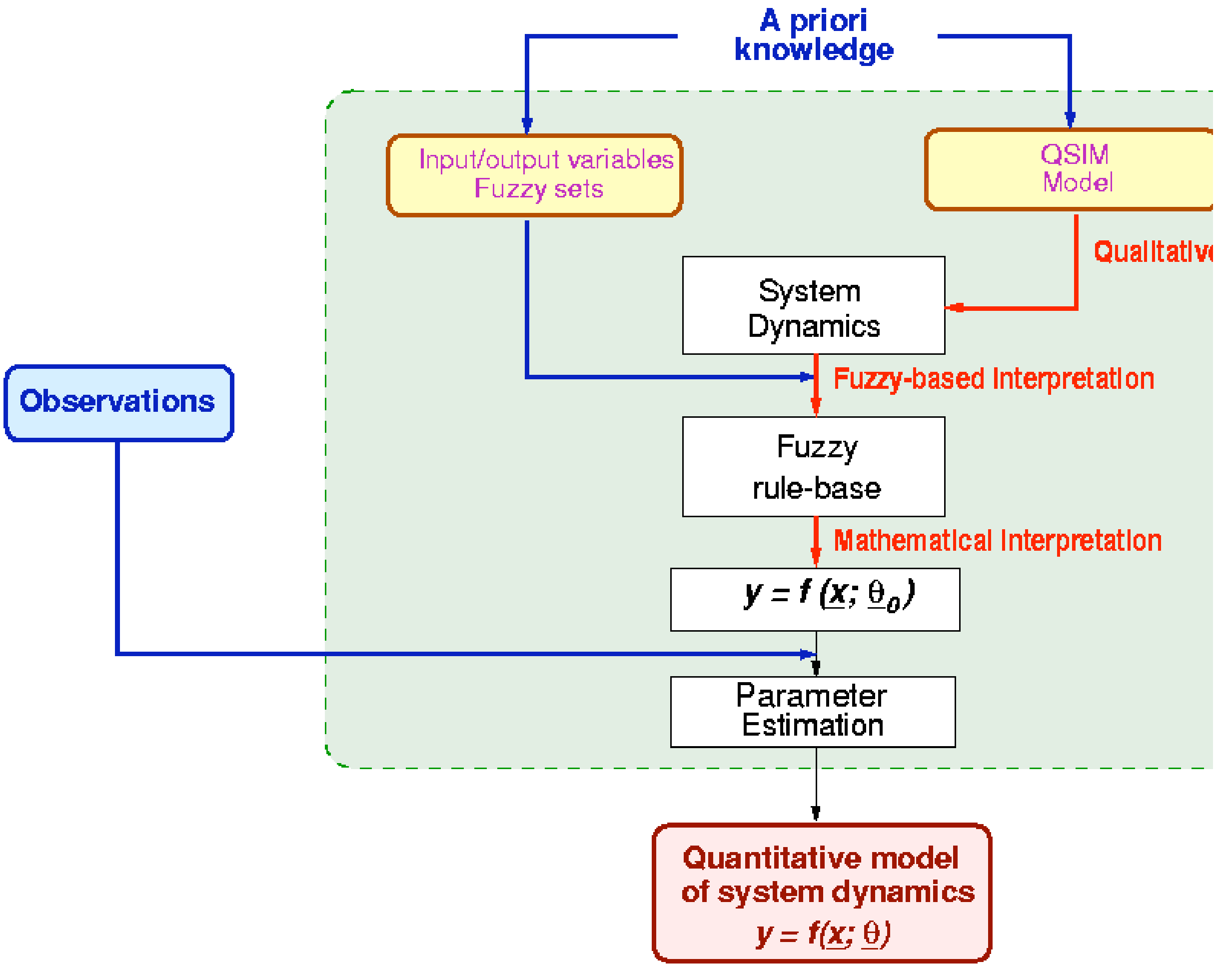

Figure 14 – *Black box systems: Main steps of FS-QM*

5. Conclusion and open issues

This paper 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 paper is not intended at a comprehensive overview of QR. Some important aspects have been left out like *causality,* which is crucial as soon as we want to explain the behavior of a system [28][17]. But the presented concepts and tools show that QR offers a significant modeling methodology. However, it suffers limitations that can be imputed to the generality of the proposed approaches along with the weakness of qualitative information. The first steps, illustrated in the paper, towards the development of QR methods tailored to specific classes of problems, as well as their integration with numerical/statistical methods have confirmed that unified modeling approaches may provide solutions that outperform either pure qualitative or pure quantitative ones.

The automation of the modeling process is one of the open questions, in particular how to bridge the conceptual and higher abstraction models of QR to engineering models [51]. Determining a set of relevant landmarks from the input/output of numerical 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 very local nature of numeric models.

Compositional modeling is also of great interest. For current practice in numerical 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 fragments composition. To be automated, this process calls for *influence resolution*, i.e. the process of transforming a complete set of influences on each variable to constraints, so the resulting model will support simulation. It hence requires the concept of influence and the explicit representation of the phenomena occurring when assembling two fragments. Although QR has contributed to this topic and QPT can be quoted in this respect [20][21], this remains an open issue.

6. References

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