Developments Towards Constraining Qualitative Simulation*

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In recent years, qualitative reasoning with physical mechanisms based on qualitative differential equations (QDEs) has emerged as a major line of research. In particular, de Kleer, Forbus and Kuipers have developed powerful qualitative simulation techniques to obtain solutions for these equations. These techniques derive behaviors causally from structures given. They handle intuitive models and incomplete knowledge. In writing about his qualitative simulation algorithm [Kuipers86], QSIM, Kuipers pointed out that the algorithm generates all behaviors of a mechanism given its qualitative description: "that all actual behaviors of a mechanism are predicted by its qualitative simulation". However, he also pointed out that the algorithm "cannot be guaranteed against producing spurious behaviors: behaviors which are not actual behaviors for *any* physical system satisfying the constraint equations". Furthermore, he pointed out that this problem does not occur with the QSIM algorithm alone, but "also occurs with the algorithms of de Kleer and Forbus". Thus, careful analysis is required before solutions produced by qualitative simulation can be put to use. This limitation seriously reduces the appeal and usefulness of these powerful tools and thus the systems on which they are based.

The simple spring as described by the following QDE:

$$a = M_0^-(x)$$

where M_0^- denotes a monotonically decreasing function of x passing through 0 at $x = 0$,

x denotes the displacement of the point mass at the end of the spring from its natural resting position,

and $a = \frac{d^2x}{dt^2}$ is the acceleration of the point,

has one qualitative behavior — a steady oscillation. However, on simulating the system for one period of oscillation, QSIM predicts three possible behaviors (Figure 1), corresponding to a diminishing oscillation, an expanding oscillation and a steady oscillation (Figure 2). A simple energy analysis of the system eliminates the diminishing and expanding oscillation cases. The analysis is as follows:

- • Denotes a state all of whose possible subsequent states have been generated.
- ◉ Denotes a state that is either identical to one of its ancestors (forming a cycle) or is quiescent (all derivatives zero).
- ○ Denotes a state none of whose possible subsequent states have been generated.

Figure 1: Behavior Tree of Possible Behaviors of the Simple Spring Predicted by QSIM

Multiplying the QDE through by $v\,dt$ gives:

$$av\,dt = M_0^-(x)v\,dt$$

$$\frac{dv}{dt}v\,dt = M_0^-(x)\frac{dx}{dt}\,dt$$

$$v\,dv = M_0^-(x)\,dx$$

Integrating on both sides from $t = 0$ gives:

$$\int_{V^*}^{v} v\,dv = \int_0^x M_0^-(x)\,dx$$

$$v^2 - V^{*2} = \int_0^x M_0^-(x)\,dx$$

$$v^2 - \int_0^x M_0^-(x)\,dx = V^{*2}$$

This implies the constraint: $x = 0 \iff v = \pm V^*$. Since states 9 and 10 in Figure 2 violate this constraint, their corresponding behaviors are not genuine. Only the steady oscillation is.

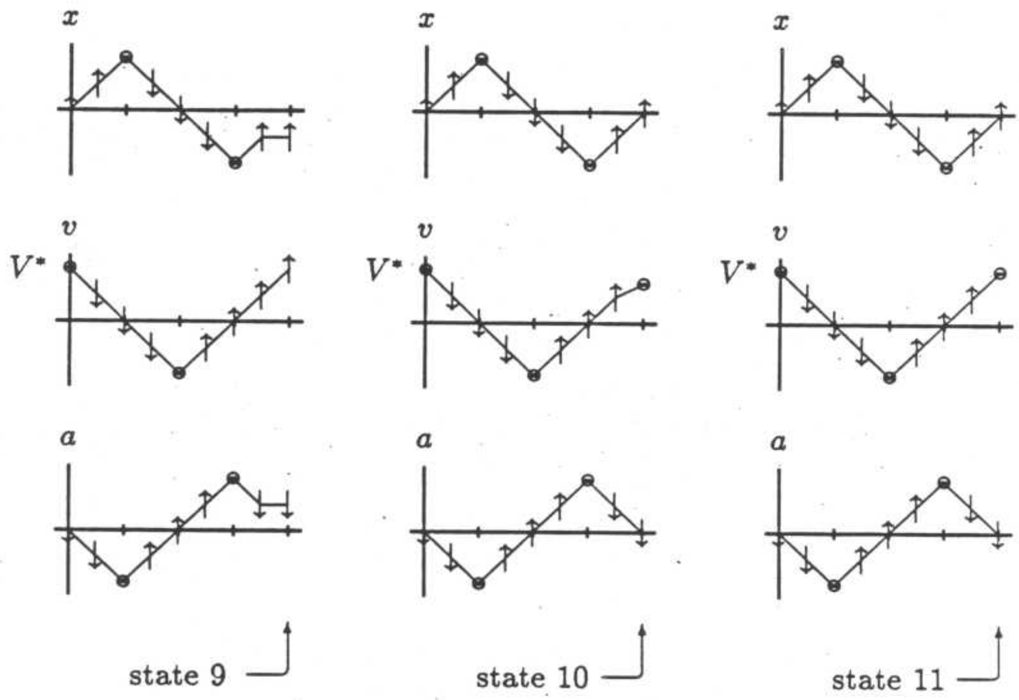

Figure 2: Behavior Plots of Possible Behaviors of the Simple Spring Predicted by QSIM

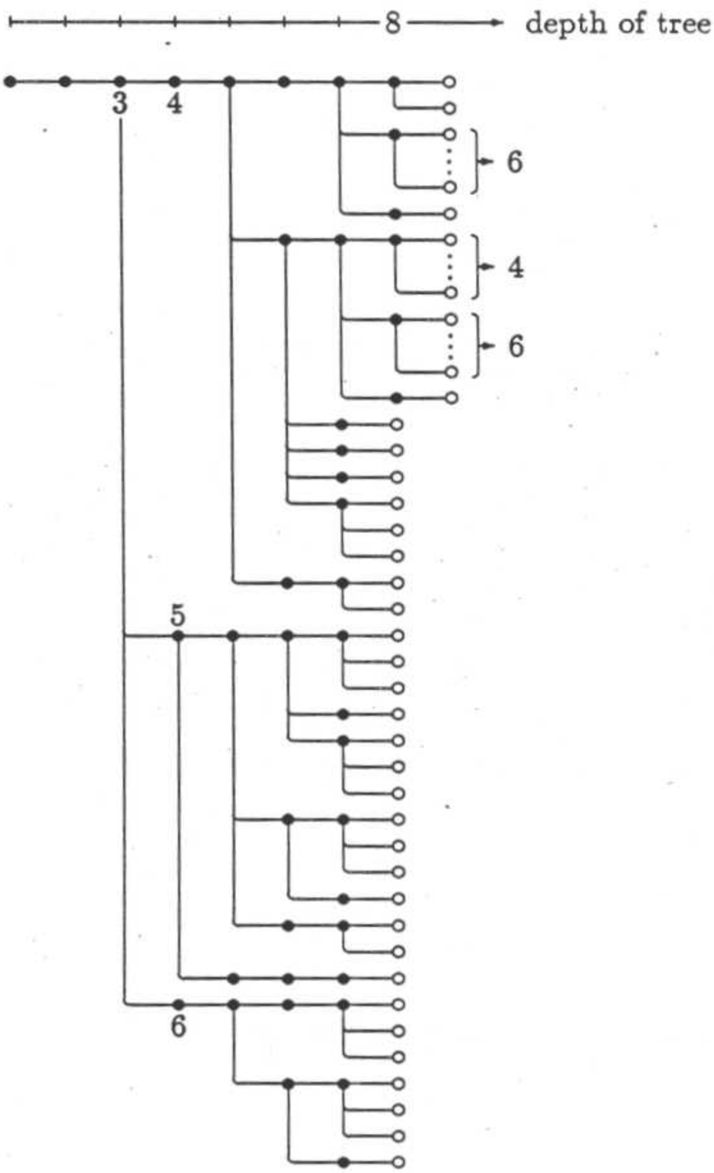

Figure 3: Initial Behavior Tree of Damped Spring

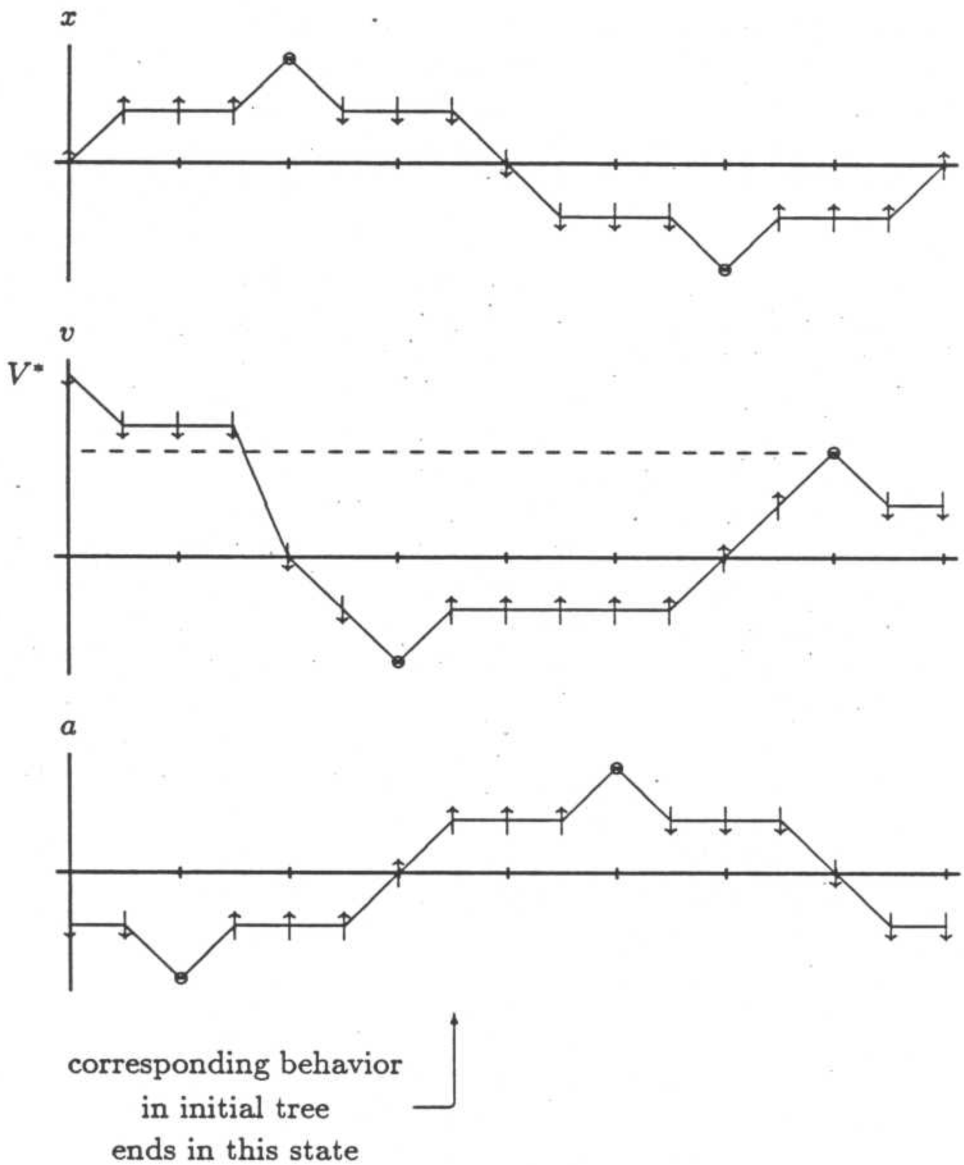

Figure 4: Behavior Plot of Damped Spring

Such post-simulation analysis suffices to identify the genuine behaviors of simple systems such as the simple spring. However, it turns out to be inadequate for more complex systems such as the damped spring, described by the following ordinary differential equation (ODE):

$$ma = -kx - \eta v$$

Initial simulation of the damped spring by QSIM for 100 states gives the apparently unmanageable behavior tree of Figure 3. It can easily be noticed that the tree branches exponentially. If we assume that there are relatively few genuine behaviors, many of the branches would be spurious. Thus, rather than letting the spurious branches propagating through the tree and multiplying (making the tree unmanageable), it is necessary to eliminate them as they are generated. In our work, we applied simple analysis (similar to what is applied to the simple spring) to obtain three types of constraints which when applied to the simulation of one period of oscillation of the damped spring, gave the one single genuine behavior of the system (Figure 4). Some arbitrary initial condition was used. The three types of constraints are the second derivative constraint, the extremum constraint and the system properties constraint.

In reference to QSIM producing spurious behaviors, it was pointed out that "the underlying problem is the combination of locality with qualitative description" [Kuipers86]. The process of simulation is inherently local in that successors to a state are computed given only information in that state. No global information is used explicitly in the process, only what is encoded implicitly in terms of parameter values. In a numerical simulation, excluding truncation errors, global information is captured fully through the use of numerical values in the form of differing parameter magnitudes. No ambiguity results. In the case of qualitative simulation, magnitude information is only partially captured. For example, the value of a changing parameter over a time interval is described only as lying between two adjacent lankmark value. Such qualitative description cannot be used to capture a global property such as total system energy that is computed from the changing values of position and velocity. The extremum and system properties constraints address this type of problems. They capture global information already present in the given description, but which is not utilized by the simulation. The extremum constraint is essentially an energy constraint whereas the system properties constraint specifies that the relationship between km and η^2 of the ODE (one of $<$, $=$ or $>$) be constant.

Insufficient use of derivative information in the QSIM algorithm also contributes to the generation of spurious behaviors at a local level. Within QSIM, only the first derivative of each parameter is taken into account explicitly. When the first derivative vanishes, however, the second derivative is needed to make local predictions [deKleer84]. Its unavailability causes QSIM to branch on all possibilities of the first derivative in the next state, giving rise to spurious behaviors. Our second derivative constraint addresses this problem.

At first glance, it may seem possible to eliminate the need for a second derivative constraint by making second derivative information explicit. However, this turns out *not* to be the case. Second derivative information is needed only when the first derivative vanishes. Detailed specification of all possible values of the second derivative throughout the simulation would only lead to unnecessary proliferation of possible states, and thus possible behaviors.

In view of the success with the simple and damped spring on the QSIM system, the constraint derivation approach towards accounting for spurious behaviors generated during qualitative simulation appears promising. Thus far, the approach has been shown to work with second order ODEs with constant coefficients using three types of constraints. Extending the approach to work with a second order QDE also yielded useful results despite the "looseness" of QDEs. However, more work is needed to see how far the approach can be taken. A goal for continuing research in this direction is the construction of a system which would do the foregoing analysis automatically given a structural description of a mechanism (in terms of either ODEs or QDEs). Constraints resulting can thus be used by a modified qualitative simulation system which utilizes them to keep itself from producing extra behaviors. Attempting to construct such a system raises many questions. They include:

- Is the QSIM structural description language "at the right level" in the sense that the language can be used to describe a large class of systems in a useful way? If not, what would be an appropriate one?

- How does the language used affect the analysis required to derive constraints?

- Given a structural description of a system, do constraints exist that would guide simulation appropriately?
- Given that they do, how do we identify what they are?
- How can we be sure that the constraints filter out *all* and *only* the spurious behaviors?
- ⋮

Work has been continuing in these general directions. Further progress will be reported.

References

1. J. de Kleer and D. G. Bobrow. 1984. Qualitative Reasoning with Higher Order Derivatives. *Proceedings of the Fourth National Conference on Artificial Intelligence (AAAI-84).* Los Altos, CA: William Kaufman.
2. B. J. Kuipers. 1985. The Limits of Qualitative Simulation. *Proceedings of the Ninth International Joint Conference on Artificial Intelligence (IJCAI-85).* Los Altos, CA: William Kaufman.
3. B. J. Kuipers. 1986. Qualitative Simulation. *Artificial Intelligence* **29**: 289–338.
4. W. W. Lee, C. Chiu and B. J. Kuipers. 1987. Developments Towards Constraining Qualitative Simulation. Technical report in preparation.
5. D. Weld. 1986. The Use of Aggregation in Causal Simulation. *Artificial Intelligence* **30**: 1–34.

Title QUALITATIVE PHYSICS APPLIED TO A DEPROPANIZER IN PROCESS CONTROL

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Abstract

A good understanding of the physical phenomena is the basis of an efficient control of a process by the human operator. This is why operators are taught a qualitative model of the process. It relies on synthetic and operational parameters. We have built a Qualitative Physics Model, by formalizing and enhancing this pedagogical model. We describe this Qualitative Physics Model then we show how it can be used in diagnosis to find the causes of a perturbation, as well as in prevision to forecast and give a justification of the evolution that follows a perturbation. A monitoring system which integrates these functionalities is under development.