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Combined Qualitative and Numerical Simulation with *Q3**

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Abstract

Combining numerical and qualitative simulation into one technique allows simulation to be performed even when there is insufficient information for a numerical simulation. Predictions are also guaranteed correct. Also, numerical simulations predict just one behavior; combined simulations can predict more than one when this is warranted. Thus, combined simulation is an improvement over numerical simulation.

Combined simulation is also an improvement over qualitative simulation. Qualitative simulation provides weak predictions, because it relies on weak model descriptions. Combined simulation allows adding numbers to model descriptions, resulting in stronger and potentially more practical predictions.

Q3 is a system for doing combined simulation. It uses intervals to express partial information about values, because intervals can express values anywhere from fully specified numbers, to partially specified numbers, to very vague qualitative values. Q3 also explicitly represents qualitatively significant values, like qualitative simulation, and other values, like numerical simulation. Thus, Q3 represents, and reasons, in ways that neither numerical simulation nor qualitative simulation do alone.

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1 Introduction

Simulation of continuous systems has a long history and much practical use. Historically, such simulation has come under the heading of numerical methods. More recently, Artificial Intelligence has entered the field with *qualitative simulation*, pioneered by de Kleer [1977, 1984], Forbus [1984], and Kuipers [1984, 1986].

Qualitative models can represent a *class* of system, because real systems that are only partially equivalent to each other can correspond to the same qualitative model. This is in contrast to the complete system specifications typical of numerical models. The desire to model and simulate a class of systems can be a reason for choosing qualitative modeling and simulation.

Another reason for using qualitative modeling is that information precise enough for a numerical model may not be available. This lack of information need not prevent modeling a system, or force the use of arbitrarily chosen "reasonable" numbers, because qualitative modeling could be a reasonable option when complete information is not available.

Thus, qualitative modeling and simulation has advantages over numerical methods. However there are disadvantages as well. The weak specifications inherent in a qualitative model can cause a simulation to be unable to predict very far into the future before encountering a state with more than one and perhaps intractably many possible futures. Also, the predictions of a qualitative simulator are weak compared to numerical simulations. These problems with qualitative simulation are alleviated by introducing quantitative information into the model. Even partial quantitative information, such as intervals, is helpful. This is why we wish to be able represent our models with however much or little information we have about them. Intervals are useful for this because they can represent a wide range of partial information.

Work on adding numerical information to qualitative models and simulations has been reported previously, for example by de Kleer ([1975], [1977]), Simmons [1983], Forbus [1986], Williams [1988] and [Kuipers and Berleant, 1988]. These researchers and others succeeded to varying degrees in integrating quantitative and qualitative information. However, that work maintained qualitative and quantitative knowledge in distinct representations, integrating them by mediating between the two representations. When combining qualitative and quantitative information in a single model, we wish to use just one representation, in the interest of representational and inferential simplicity. The work presented here describes a system, **Q3**[1], that goes beyond previous work on mediating between qualitative and quantitative simulations, by producing hybrid simulations with characteristics of both numerical and qualitative simulations, and also by using a single representational framework which supports expressing information anywhere on a spectrum from

[1] Q3 is a superset of a previous system, Q2 [Kuipers and Berleant, 1988], which in turn is a superset of QSIM [Kuipers, 1986]. We will often use the term Q3 here even when the terms Q2 or QSIM could have been used instead.

qualitative values to single numbers.

Let us look at examples of **a)** qualitative simulation, **b)** qualitative simulation with added numerical information and its converse **c)** numerical simulation with added qualitative information, and finally, **d)** combined qualitative-and-quantitative simulation. We do this using a cycling thermostat system model: The state of a cycling thermostat system changes continuously except for occasional abrupt transitions when the thermostat turns `ON` or `OFF`. Such a system needs to be simulated by a technique that handles not only continuous systems, but also a generalization: Continuous systems with discontinuities. Q3 can handle this, so we chose to model the cycling thermostat system to illustrate the research presented here.

Intuitively, the temperature of a living unit in hot weather will rise at a rate depending on the thermal mass of the air in the living unit, the amount by which the outside temperature exceeds the inside temperature, and the thermal resistance of the boundary between inside and outside. When the inside temperature gets high enough, the thermostat transitions to `ON`, and the air conditioner pumps heat outside. The temperature change is now also a function of the air conditioner cooling capacity. Normally this function results in a decline in living unit temperature, until the thermostat transitions to `OFF` and the cycle repeats.

2 Qualitative Simulation

A qualitative simulation of the cycling air conditioner system is shown in figure 1. Note that all qualitatively significant values for time and the other variables are named. `T0` is when the simulation starts. At `T1` and `T3` the thermostat trips `ON` or `OFF`. At `T2` the inside temperature equals the thermostat setting. Symbolic names for values of the other model variables are shown also. These values appear on the vertical axes of the plots. Figure 1 shows the normally operating system in which the inside temperature gets warmer until the air conditioner turns on, then the air gets cooler until it turns off, and the cycle repeats.

The simulation also produces several other possible behaviors; each corresponds to a branch of the behavior tree in the upper right corner of the figure. For example, perhaps the outside temperature is warmer than the thermostat setting, but only slightly. Then, the indoor temperature slowly rises asymptotically toward the outside temperature, but never gets high enough for the air conditioner to turn on.

3 Qualitative simulation with quantitative information added.

By adding quantitative information, even incomplete quantitative information that is insufficient for a numerical simulation, quantitative inferences may be reached about various qualitative values in a simulation. In Q3, these inferences are done by constraint propagation among model variable values.

For example, consider one of the constraints in the cycling air conditioner model: `((mult R HFin dTemp))`. This constraint declares that the temperature difference between inside and outside, dTemp, equals the resistance of the living unit to heat flow in or out, times the rate of heat flow occurring despite that resistance. This constraint must hold at all times. One of its instantiations in the behavior shown in figure 1 is $R6 * IF29 = IO29$. In Q3 such constraints, determined by the model and behavior, are used to filter the possible quantitative values of the (three in this case) qualitative values constrained. Constraint propagation with interval labels was examined by Davis [1987]. When doing the propagation, a value is expressed as an interval arithmetic expression in terms of the other values of the constraint. This expression is evaluated using the rules of interval arithmetic (see for example [Moore, 1979] and [Alefeld and Herzberger, 1983]). The result is intersected with the current label and the intersection assigned as the new label. Davis [1987] argues that constraint propagation with interval labels is correct. For a more rigorous proof see Berleant and Kuipers [1990].

These inferences may allow other higher level conclusions [Kuipers and Berleant, 1988], such as:

•— Ruling out behaviors. For example, inferring that a parameter is both in the interval $[1, 2]$ and $[5, 10]$ means the behavior can be ruled out, because a value of a parameter cannot be within disjoint intervals simultaneously. If all behaviors of a model can be ruled out, the model is ruled out.

•— Making predictions about unknown values. The constraints among values imposed by the model and behavior allow quantitative knowledge about some values to be used to make inferences about the quantitative values of some or all other qualitative values.

These conclusions are illustrated in figure 1.

4 Full-spectrum representation and hybrid simulation.

A simulation which expresses and uses values that are either qualitative, numerical, or expressed both ways simultaneously will be termed *hybrid*. A representation which can express data anywhere on a continuum between completely specified numerical information, and qualitative information will be termed *full-spectrum*. Let us look at *hybrid* and *full-spectrum* in more detail.

4.1 *Hybrid* simulation

By *hybrid* we simply mean that the simulation can express and use values expressed qualitatively, numerically or both. An example is shown in figure 2, which has characteristics of both a qualitative simulations and a numerical simulation. In figure 2, both qualitative and numerical values are represented. The transitions between the `air-conditioner-ON` and

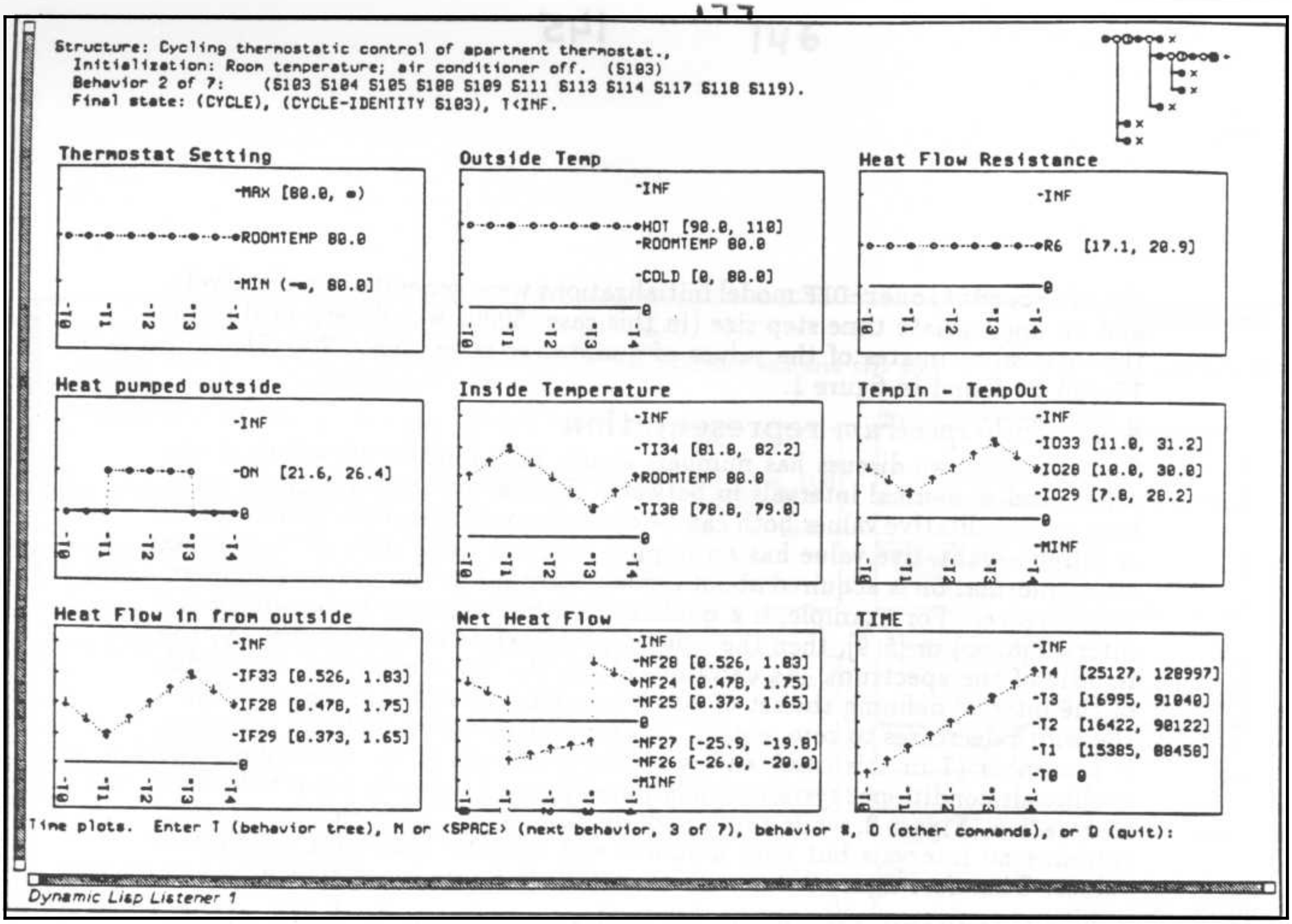

Figure 1: Simulation of the air conditioner system: If no quantitative information was added, none of the intervals would be shown, and all seven behaviors would be plausible. With partial quantitative information, six behaviors can be ruled out (marked with an X), and quantitative inferences are made.

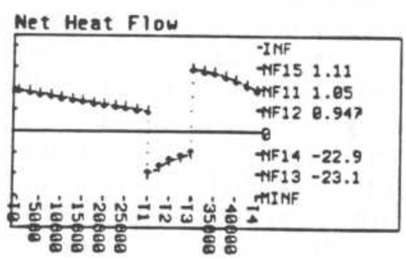

Figure 2: Hybrid simulation of the cycling air conditioner system, showing one of the model variables.

the `air-conditioner-OFF` model initializations were generated qualitatively, and an appropriate time step size (in this case, 5000) was determined using the interval estimates of the values of qualitative time points **T0**, **T1**, **T2**, **T3** and **T4** found in figure 1.

4.2 *Full-spectrum* representation

The spectrum we discuss has numbers at one end, qualitative values at the other, and numerical intervals in between. This a continuum because numbers and qualitative values both can be viewed as extremes of interval widths. A purely qualitative value has an implicit interval value such as $(0, \infty)$. As more information is acquired about a qualitative value, the width of its interval decreases. For example, if a qualitative value is known to be within the interval $[5, \infty)$ or $[5, 9]$, then the value representation is moving through the middle of the spectrum. As certainty about the value increases, the width of the interval defining the set of possible numerical values decreases. When the width decreases to zero, e.g. $[7, 7]$, the value is known with full certainty, is a number (7 in this case) and is at the other end of the spectrum. The cycling air conditioner system simulation of figure 1 uses a full-spectrum representation. Figure 2, while a hybrid of qualitative and numerical simulation, contains no intervals but only numbers and symbols indicating qualitative values. Therefore figure 2 does not use a full-spectrum representation.

4.3 Bridging the gap: A full-spectrum, hybrid simulation.

A simulation of the cycling air conditioner which is both hybrid and full-spectrum appears in figure 3. For a very si[illegible]ed in much greater detail see Berleant [1989].

Note that there are now some new symbols with associated intervals, such as **K8**. These symbols are not qualitatively important — yet they can still be represented. In addition, many intervals exist in internal data structures but, for readability, are not explicitly printed. For example, the plot for model variable **Heat Flow in from outside** has intervals associated with all 19 time points. The midpoints of unprinted intervals are used to determine plot coordinates as the curve goes from **T0** to **T4**.

The scales of the plots in figure 3 need some explanation, as (except for **Outside Temp**) they are not to scale. Labeled values are equally spaced along the axes of most plots, regardless of their associated intervals. Between the labeled values, the unlabeled values are plotted to scale. But, since the scale is usually different between different pairs of labels, the curves are distorted. When the plots of figure 3 are all plotted with constant scales, the resulting curves look different. For example, **TempIn - TempOut** looks like figure 5 (except for the interval labels).

4.3.1 Correctness of the inferred ranges.

By *correct* we mean that any real mechanism satisfying the structure and initial conditions of the model will exhibit values within the intervals inferred

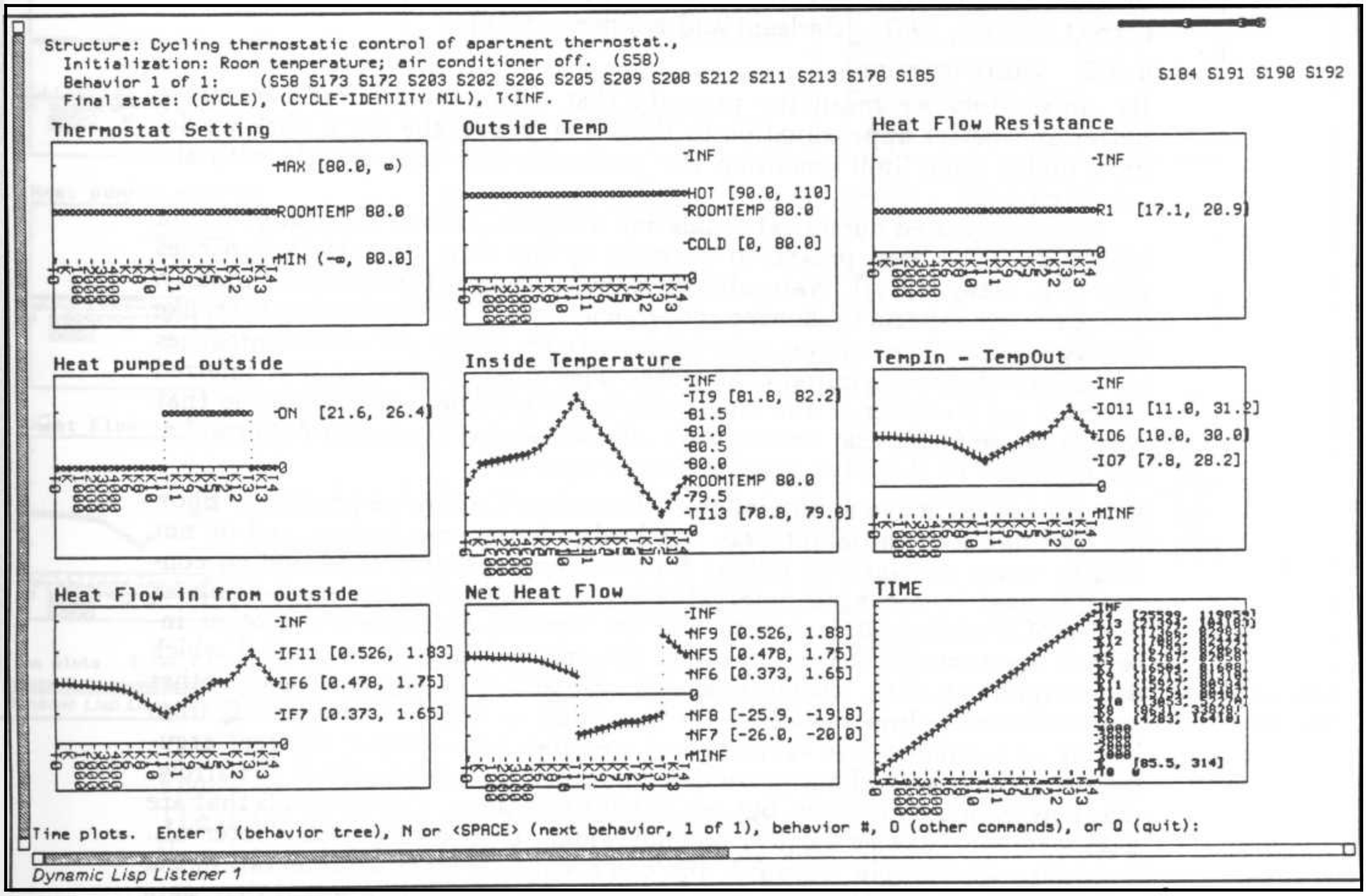

Figure 3: A combined hybrid, full-spectrum simulation of the cycling air conditioning system. The initialization is the same as for figure 1.

by Q3. Q3 is correct because constraint propagation with interval labels is correct ([Davis, 1987], [Berleant and Kuipers, 1990]).

4.3.2 Convergence

By *convergence* we mean the property that a simulated curve becomes a better and better approximation to the actual curve, the more work we do, until under some limit condition the prediction coincides exactly with the actual curve.

Commonly used numerical simulation methods, such as the Runge-Kutta technique, have been proven to converge as the time step size approaches zero (e.g. Gear [1971]). Naturally we want to know if Q3 behaves similarly. There are two aspects to showing convergence in Q3. One is showing that, like the Runge-Kutta technique, convergence occurs as the step size approaches zero — given precise initial conditions. The other is showing that inferred intervals get narrower as the initial conditions become more precise, so that we can be confident that narrower initial intervals lead to better final results. We now look at these two aspects of convergence.

Inferences improve as initial conditions become more precise. Showing that narrower initial intervals can lead to better conclusions, and do not lead to worse conclusions, follows from the *implausibility* condition on constraints used to propagate interval labels: Numbers that are implausible as values of a constraint argument will not become plausible when other intervals are narrowed. Let C be any constraint and Q be a symbol which is an argument of C. Define *adjacent* such that Q is *adjacent* to the other arguments of C. Implausibility says that numbers which C disallows Q from having as a quantitative value, cannot become allowed when adjacent arguments are narrowed. Thus narrowing the initial intervals can lead to narrowing their adjacent intervals, but not to widening them. Any intervals that are narrowed can likewise narrow, but not widen, their own adjacent intervals. This narrowing ripples outward, and can eventually reach all intervals in the constraint network. Unfortunately, cycles can occur when intervals that were narrowed once before become narrowed again, and again, and again. This could lead to non-termination. Luckily non-termination is not hard to prevent, although halting computation means not finding the narrowest possible intervals [Davis 1987].

Figure 4 shows the inferences that can be made when the initial conditions to the combined hybrid, full-spectrum simulation of figure 3 are narrowed all the way to single numbers. Comparing the figures, it is clear that the inferred intervals tend to be markedly narrower. Most of them are numbers, the narrowest possible intervals. Figure 5 shows one of the model variables plotted using a constant scale.

Convergence and time step size. Most numerical simulation techniques, such as the Runge-Kutta method, give more accurate results as the step size of the independent variable (e.g. ΔT) decreases. Likewise, note the improved, narrower intervals achieved for the combined simulation (figure 4)

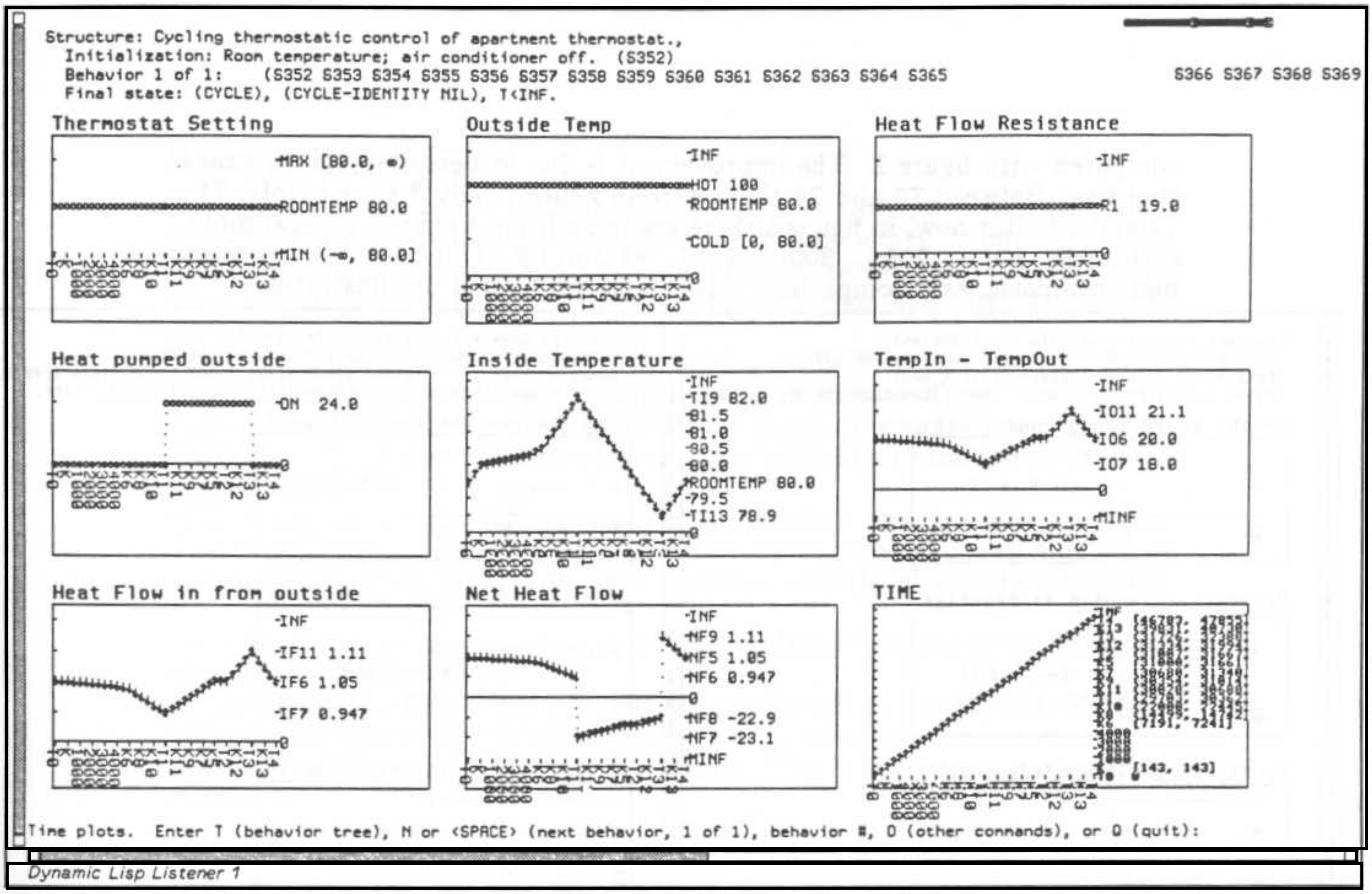

Figure 4: A combined simulation of the cycling air conditioning system. The initial quantitative information is specified as individual numbers rather than intervals as in figure 1. Each initializing interval in figure 1 has been replaced by the number at the middle of that interval, thus initializing HOT, ROOMTEMP, TI9, TI13, ON and R1.

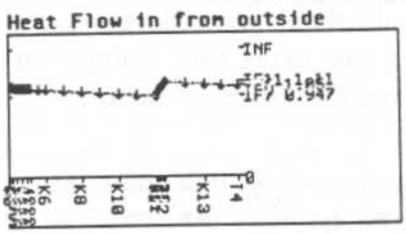

Figure 5: A model variable from figure 4, plotted with constant scales for the axes.

compared with figure 1. The improvement is due to decreasing the average step size: Between T0 and T4 there were in figure 1 only 3 time points, T1, T2 and T3. But now, in figure 3 there are in addition to those, several more, such as K, 1000, 2000, 3000, 4000, K6 and K8. This narrowing is often more dramatic, as a comparison between figures 6a and 6b illustrates.

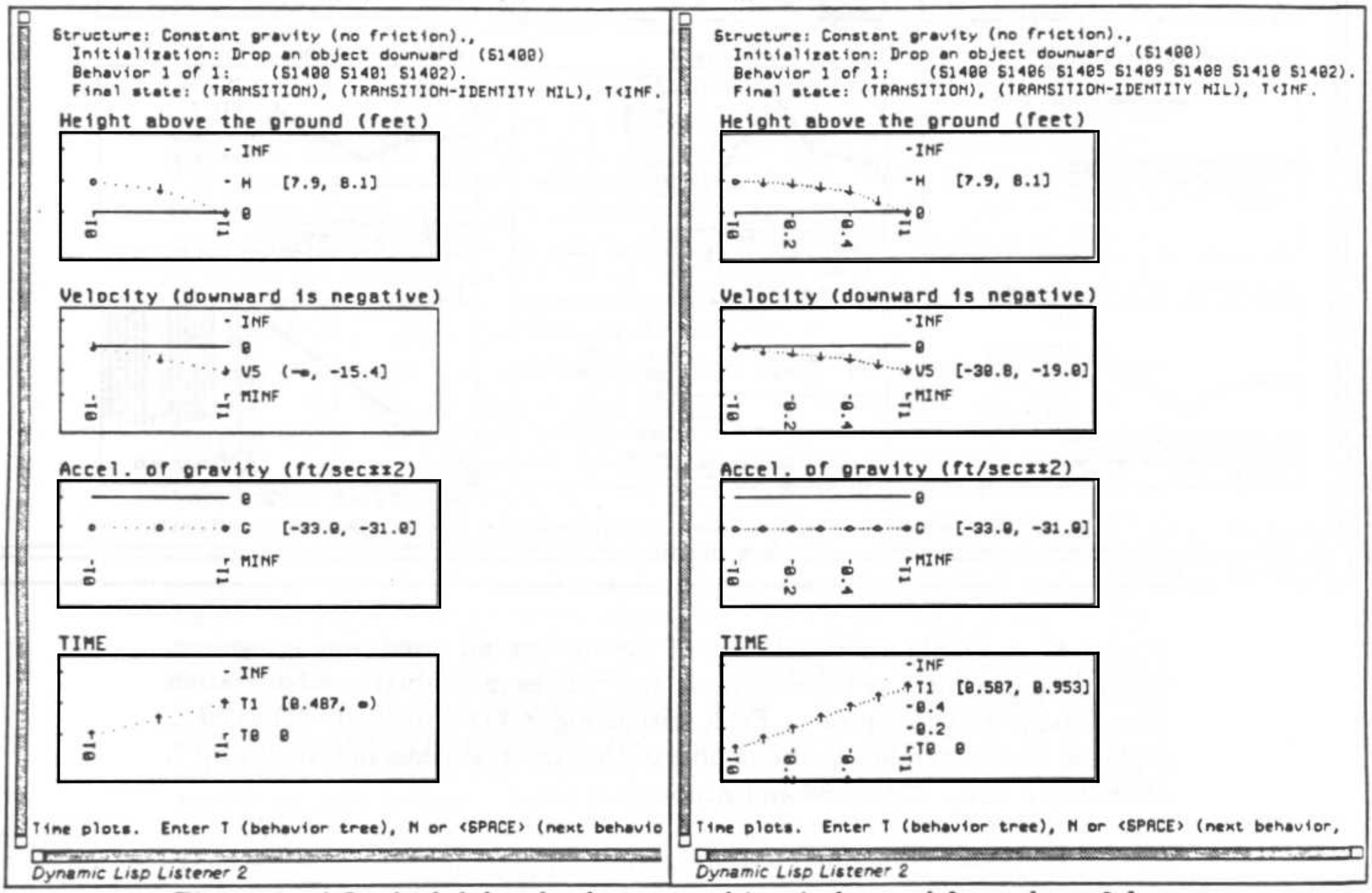

Figure 6: **a)** In the left hand column, an object is dropped from about 8 feet. In **b)**, in the right column, two extra time points were inserted, leading to much better inferences about the values of V5 and T1.

It is not surprising that inserting time steps into a simulation improves the resulting inferences, because the total number of constraints that Q3 uses to do constraint propagation increases when time steps are added in. This is because each constraint template that is part of the model definition is instantiated for the values of the model variables at all the time points. Therefore when there are more time points there are more constraints.

5 Conclusions

Combined simulations have the following theoretical and potentially practical properties (illustrated by figure 3), that other approaches do not have:
•Hybrid simulation provides a conceptual bridge between two seemingly distinct approaches to simulation: Numerical simulation and qualitative simulation.
•Full-spectrum data expressibility provides a conceptual link between seemingly distinct representations: Qualitative and numerical. Thus, full-spectrum data expressibility bridges the gap between qualitative and numerical representations. Intervals, of course, are only one approach to full-spectrum data expressibility.
•Q3 implements both full-spectrum representation and hybrid simulation. This truly bridges the gap between qualitative and numerical reasoning about continuous systems, in both the representation and the algorithmic domains.

Combined simulations also have some major derivative properties of significant potential practicality:
•Partial initial quantitative information is sufficient to run the simulation.
•Qualitatively different behaviors are retained if they are consistent with the initial conditions, and represented explicitly. This is in contrast to numerical simulators.

Finally, the combined simulation technique described here has other derivative properties that are interesting and potentially useful.
•Transitions between simulation models are generated automatically.
•Time step sizes need not be constant.
•Qualitatively distinctive points on the plots are named and given numerical bounds.
•Inferred bounds are guaranteed correct (even with non-linear models).
•Convergence is likely.

6 Future work: Applications

One intent of the combined hybrid and full-spectrum technique described here is to bring the ability of qualitative simulation to generate all behaviors to bear on real world problems.

Take an example from the field of finance. A common problem is determining the feasibility of a goal given certain initial assumptions such as interest rates. Unfortunately the exact values of such input parameters often cannot be known ahead of time with desired precision. Thus, there is the necessity of simply trying numerical simulations with various combinations of plausible input condition values, to find out what different behaviors are possible or to get an idea of how feasible the desired system behavior (usually, ultimately making a profit) might be. This is not only tedious, it may be impossible from a practical viewpoint to try all desired combinations of plausible values for several or many input parameters. Combined simulation will help in such a task by allowing intervals to be given as values of the input parameters, running the simulation, and observing which behaviors occur.

A similar application in engineering relates to necessary tolerances of various model parameters. Simply simulating many times with different combinations of plausible model parameter values is likely to be tedious, perhaps impractical, and could also miss possible and potentially serious (mis)behaviors.

This sort of tolerance analysis could also be done automatically. Given a model with precisely specified parameter values, an augmented version of Q3 could "blur" those values by replacing them with intervals within which the specified values fall. Then Q3 could run the simulation to find the possible behaviors.

Thus we expect an exciting potential for practical application of the Q3 system in the foreseeable future.

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