Qualitative and Quantitative Simulation: Bridging the Gap

Daniel Berleant
Dept. of Computer Systems Engineering
University of Arkansas
Fayetteville, AR 72701
djb@engr.uark.edu

Benjamin Kuipers
Department of Computer Sciences
University of Texas
Austin, TX 78712
kuipers@cs.utexas.edu

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Abstract

Shortcomings of qualitative simulation and of quantitative simulation motivate combining
them to do simulations exhibiting strengths of both. The resulting class of techniques is called
semi-quantitative simulation. One approach to semi-quantitative simulation is to use numeric
intervals to represent incomplete quantitative information. In this research we demonstrate se
quantitative simulation using intervals in an implemented semi-quantitative simulato
Q3 progressively refines a qualitative simulation, providing increasingl
predictions which can converge to a numerical simulation in the
correctness guarantees from qualitative and interval si
Q3's simulations are based on a technique w
itative simulation has a very coarse step siz
relatively few qualitatively distin
qualitative states,
to improve
Q3

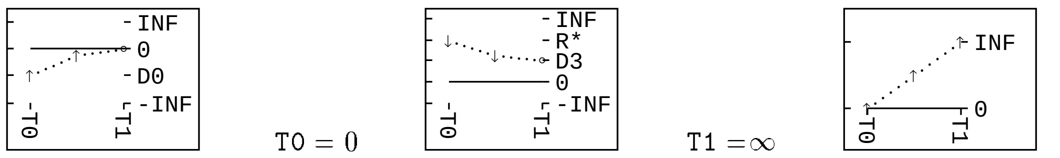
not constitut

Contents

1 Introduction

Systems that change over time are often so complex that analytical solutions, equations predicting
future system states as a function of time, cannot be found. In those cases simulation is usefu
prediction. Given a model of system structure and initial state, simulation determin
trajectory through its state space.
When accurate numerical information about structure and initial stat
of numerical simulation techniques is available. When only qual
available, a significant body of work describes methods
the many cases in which accurate numerical in
numerical simulation, yet incomplete n
for stronger predictions than
quantitative simulati
informative inf
As an ex
tion

An object is fired upward fast enough to escape a gravitational field



(a) Gravity(t) (b) Velocity(t) (c) Distance(t)

Figure 1: Qualitative simulation of an object fired upward at greater than escape velocity shows that the gravitation experienced by the object produces a negative acceleration (a), reducin velocity (b). As distance increases (c), gravitation decreases. Qualitative simulati another behavior in which the object falls back to Earth (not shown).

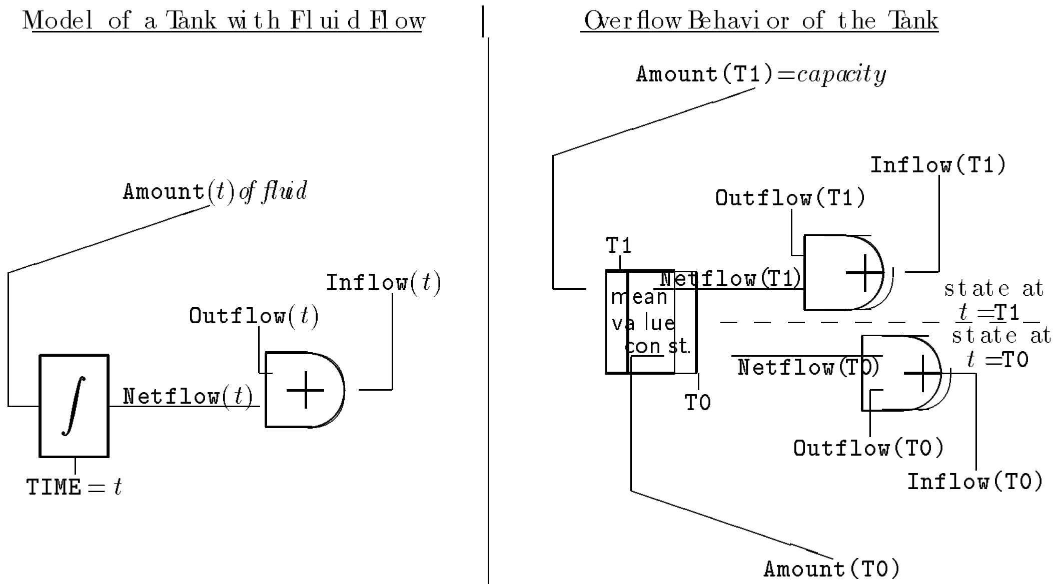
This paper significantly revises and expands a preliminary account and provides a proof of convergence and stability for step siz

2 Q3 and Step Size Refinement

Q3 improves on pure qualitative simulation by augmen inferences when quantitative information i ing behaviors, and in providing num that quantitative informatio bounding spaces of po extracting as r explici tative simulations because the qualitative features of qualitative simulation trajectories do change significantly from one time point to the next. Therefore step sizes for qualitative simulati large by definition and so numerical inferences on them tend to be weak.

Augmenting a Q2 simulation so that it has smaller step sizes can lead to quantitative inferences, just as numerical simulations can be improved (within limits imposed by the accuracy of floating point arithm algorithm for doing this. Q3 augments Q2 with the the capability of smaller step sizes.

Q3 first generates qualitative behaviors mation via Q2. Then, better inferen step size refinement and au technique. Adaptiv represent a the



$$\texttt{Netflow}(t) = \texttt{Inflow}(t) - \texttt{Outflow}(t)$$
$$\texttt{Amount}(t) = \int_t \texttt{Netflow}(t)$$

$$\texttt{Netflow(T1)} = \texttt{Inflow(T1)} - \texttt{Outflow(T1)}$$
$$\texttt{Netflow(T0)} = \texttt{Inflow(T0)} - \texttt{Outflow(T0)}$$
$$\frac{\texttt{Amount(T1)} - \texttt{Amount(T0)}}{\texttt{T1} - \texttt{T0}} \subseteq [min(\underline{\texttt{Netflow(T0)}}, \underline{\texttt{Netflow(T1)}}), max(\overline{\texttt{Netflow(T0)}}, \overline{\texttt{Netflow(T1)}})]$$

(a) Diagram & equations of a *model* | (b) Diagram & equations of a *behavior*

(c) Overflow behavior: graphical representation

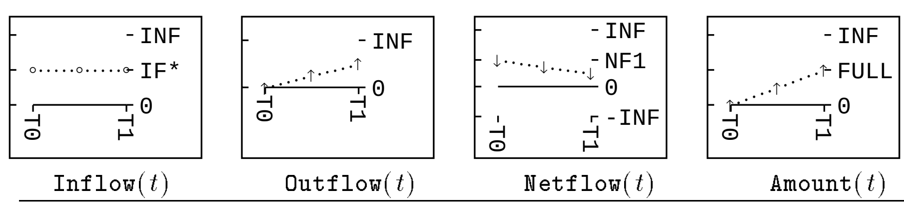
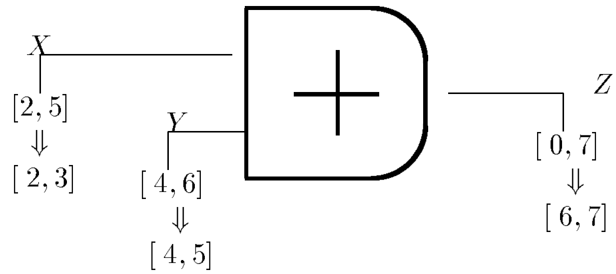


Figure 2: A simple tank model and its overflow behavior. The model consists of two const
templates, shown in (a). Those templates hold at all times. *Instantiating* the templat
tatively distinctive time points T0 and T1 leads to representations of its be
network representation of the overflow behavior is shown in (b). Al
time points would be unwieldy to depict graphically, but can
memory. The same behavior represented graphically is
quantity of fluid in the tank. Overflow occurs at
capacity of the tank. The mean value const
Amount, Netflow, and TIME.



$$Z := Z \cap (X + Y) = [0,7] \cap ([2,5] + [4,6]) = [0,7] \cap [6,11] = [6,7]$$
$$X := X \cap (Z - Y) = [2,5] \cap ([6,7] - [4,6]) = [2,5] \cap [0,3] = [2,3]$$
$$Y := Y \cap (Z - X) = [4,6] \cap ([6,7] - [2,3]) = [4,6] \cap [3,5] = [4,5]$$

Figure 3: **Constraint propagation** of interval labels through an `add` constraint. The interval at each terminal is narrowed by using the constraint to propagate the intervals currently at the other terminals, so an `add` constraint actually enforces three relations, one addition, $Z \subseteq X+Y$, a subtractions, $X \subseteq Z-Y$ and $Y \subseteq Z-X$

variables concerned at particular points in time (Figure 2b). These constraints relate in quantitatively bound the qualitative landmarks of model variables. The constr narrowing of one or more intervals (Davis 1987), where a narrower int tainty about quantitative value. When an interval is narrowed constraints directly affected can often narrow other 13). Thus the effect of narrowing an interval c the constraint network.

There are a number of different kind

- Arithmetic and monotonic c
- Greater and less than model variable
- Mean value co traje

Propa

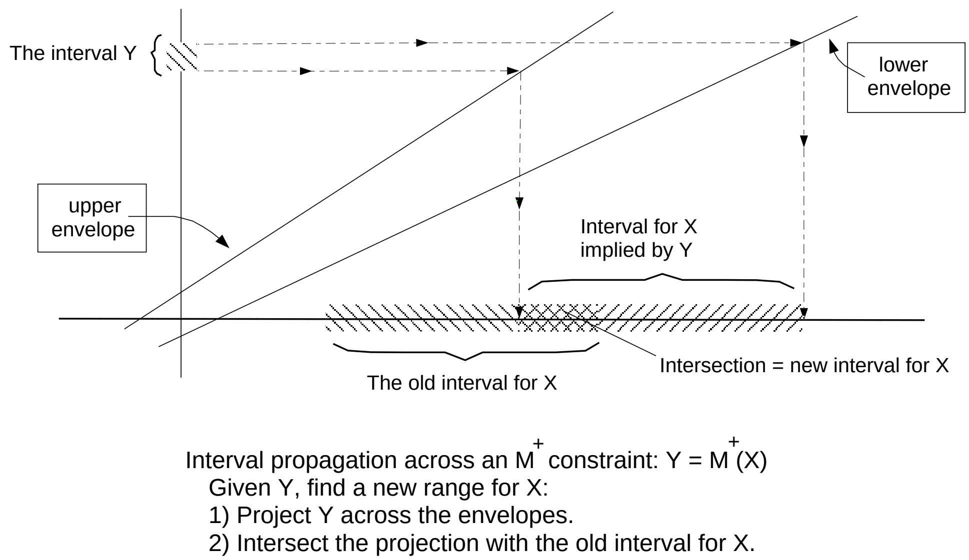


Figure 4: Propagation through an M^+ (positive monotonic) function with quantitative envelopes. Hatched regions of the axes represent intervals, and the upper and lower envelopes bound a space of monotonic functions. Propagation shown is from an interval on the y-axis to the x-axis. Propag
the other way, from x to y is analogous.

If two variables are monotonically related, the highest and lowest points of an i
them imply highest and lowest points of the projection of that interval on
A *qualitative* monotonic function represents a large set of *quan*
all those that are monotonic in the direction specified b
middle ground between qualitative monotonic func
is upper and lower monotonic *envelopes* which b
is illustrated by Figure 4, which shows a
monotonicity.

2.1.3 The mean value constraint

The mean value constraint is designed t
time point to another. It deriv
which states:

where time $t^* \in (t_{n-1}, t_n)$. r
(Forrester 1961) rel

We do not know the valu

rate(

[2] See e.g. Hyvönen (1992 p. 89–
techniques (Boltyanskii 1964).

because $t^* \in (t_{n-1}, t_n)$, because a closed interval $I = [a, b]$ is a superset of the open interval (a, b), and because the qualitative simulation module (QSIM) ensures that $rate(t)$ and all other varying quantities are monotonic between states at adjacent time points t_{n-1} and t_n.

From (1) and (2),

$$\frac{lead(t_n) - lead(t_{n-1})}{t_n - t_{n-1}} \in [\, min(rate(t_{n-1}), rate(t_n)), \;\; max(rate(t_{n-1}), rate(t_n))\,]. \qquad (3)$$

When quantities are known only to within intervals, this equation must be intervalized in the obvious ways. Real variables x_i are replaced by corresponding interval variables X_i, real func

$f(x_i)$ are replaced by corresponding interval functions $F(X_i)$, real arithmetic opera

"–" are given the corresponding interval interpretations, the natural inte

1979) of $\in$ is $\subseteq$ and functions $min()$ and $max()$ are applied respecti

bounds of intervals. Intervalizing (3) gives

$$\frac{LEVEL(T_n) - LEVEL(T_{n-1})}{T_n - T_{n-1}} \subseteq [\, min(\underline{RATE(T_{n-1})}, \underline{RATE(T_n)}), max(\overline{RATE(T_{n-1})}, \overline{R}$$

where the low bound of an interval X is denoted by $\underline{X}$ and the high bound by $\overline{X}$ (Moore 1979)

The RHS simplifies to the convex hull of the set $RATE(T_{n-1}) \cup RATE(T_n)$, or $RATE(T_{n-1}) \underline{\cup} RATE(T_n)$), where the convex hull includes everything in either interval or between them. This results in the *mean value constraint*:

$$\frac{LEVEL(T_n) - LEVEL(T_{n-1})}{T_n - T_{n-1}} \subseteq RATE(T_{n-1}) \underline{\cup} RATE(T_n). \qquad (4)$$

Equation (4) can be solved algebraically for each variable on the left hand side. The resulting right hand side can then be evaluated to give an interval, which is intersected with the quantity's current interval as in Figure 3.

Quantitative inferences provided by the mean value constraint tend to be weak when the v

T_{n-1} and T_n are widely separated, as is often the case with qualitatively distinct time

Figure 6a). Much better results are typically obtained from the mean value

size refinement, which makes adjacent time points closer together (as

Alternatives to the mean value constraint The mean value constra

method. An obvious improvement over the relatively weak Euler's

method, a mainstay of numerical simulation. For interval proble

1-step method (such as Runge-Kutta) can be extended to int

would be to use an existence and convergence theorem f

THEOREM 5.7). Moore (1979 p. 94–97) also desc

simulation. Eijgenraam (1981) and Lohne

Missuyès (1991) demonstrate the feas

simulation.

2.2 Phase II: progress

A quantitatively annotated

refined in Phase II.

which gradua

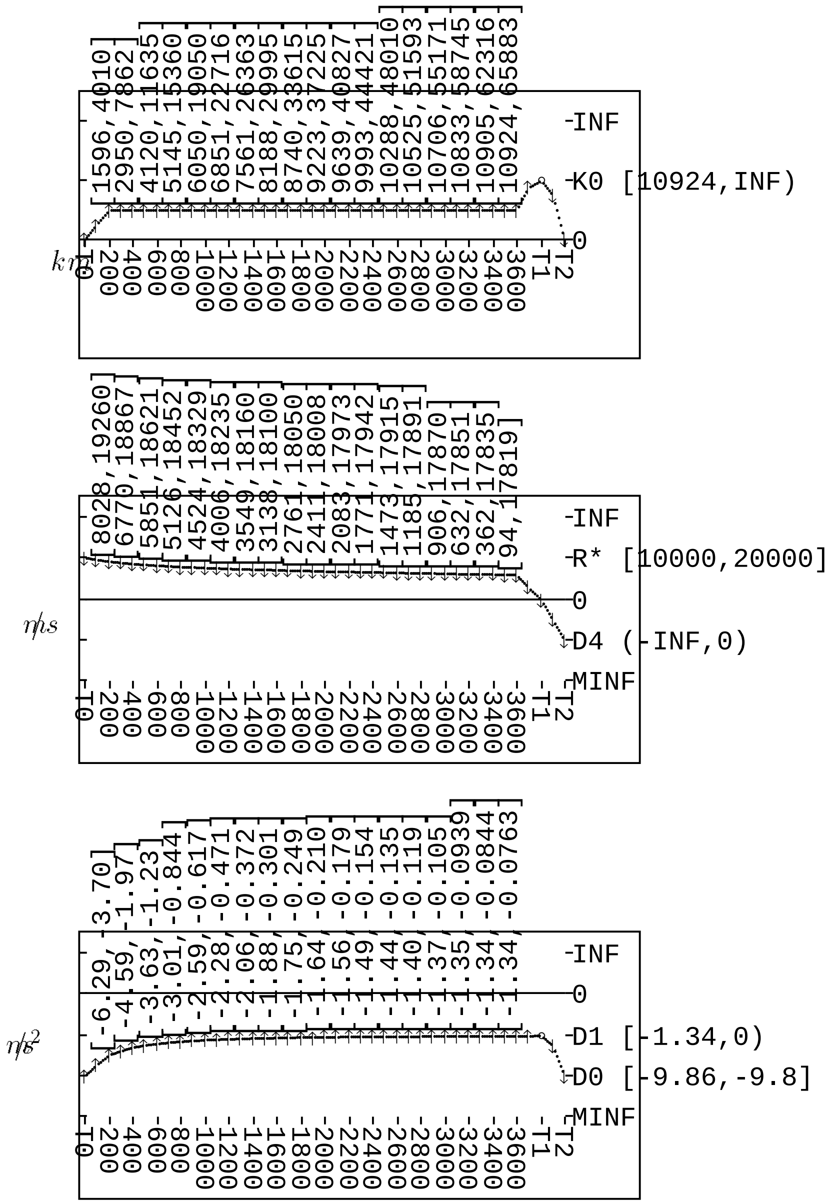
ones

2.2.1 Step size refinement: overview

Standard numerical simulation algorithms estimate system state at the next time point by ex-
trapolating from current trends. It is better to extrapolate only a short distance along the system
trajectory and then to reassess current trends before extrapolating further, than to extrapolat
a longer distance. This means keeping the step size of the simulation small and, intu
small step sizes typically lead to less error in the predicted trajectory o
For most interval generalizations of numerical simulation m
sizes lead to narrower but correct interval predictions.
step size refinement, the step sizes of the sim
sharp predictions in the form of n
These intuitions about st
proven in Appendix B

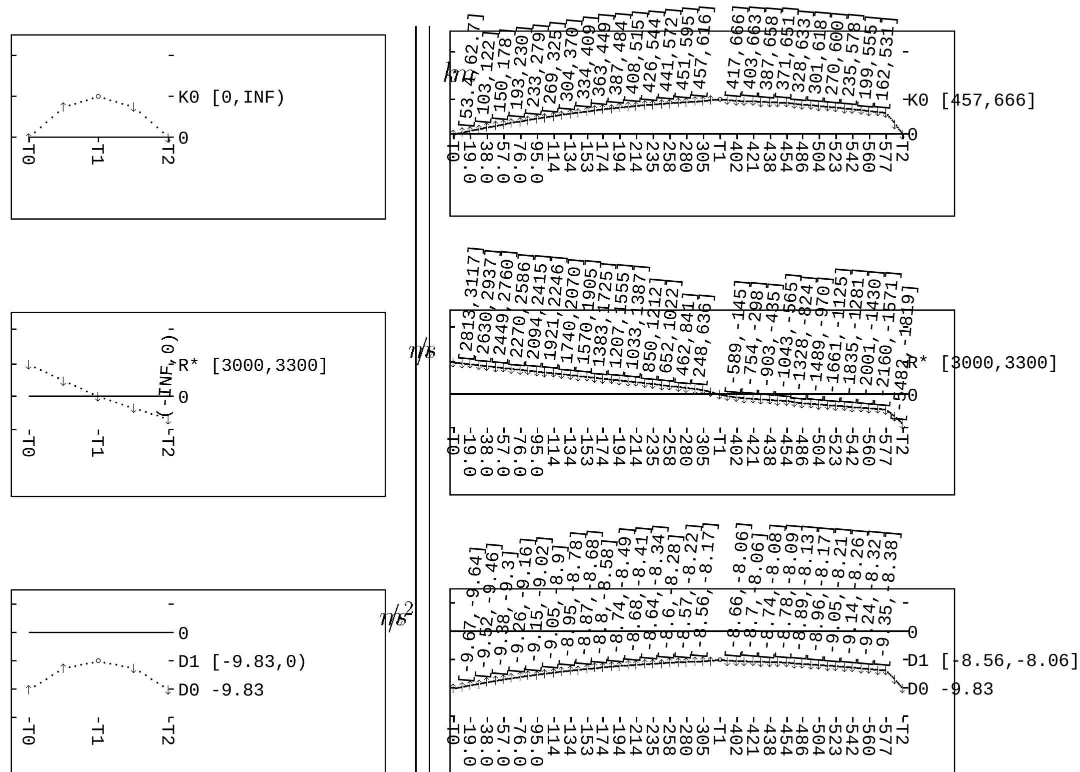
2.2.2 Step size refi

We are given a finite orde
interval range $[\underline{t_i}, \overline{t_i}$
may overla
Iter



T0 $\in [0, 0] = 0$
T1 $\in [3671, \infty)$
T2 $\in [3671, \infty)$

Figure 5: A rocket is fired upward from the Earth's surface. Gravity decreases with the squared distance from the Earth's center (Figure 8). Initial velocity is R* $\in [10000, 20000]$ $\frac{m}{s}$, which contains escape velocity (approximately 11000 $\frac{m}{s}$). Q3 correctly predicts that the rocket could either to Earth or escape. The return behavior is the one shown, with graphs for height, acceleration vs. time. Inferences about qualitative time points T0, T1, and



(a)	(b)
$T0 \in [0, 0]$	$T0 \in [0, 0]$
$T1 \in [305, \infty)$	$T1 \in [334, 384]$
$T2 \in [305, \infty)$	$T2 \in [607, 915]$

Figure 6: A rocket is fired upward at [3000, 3300] meters per second, less than escape velocity. The behavior in which the rocket falls back to the ground is shown in (a), which also shows weak quantitative inferences that were unable to prune any of the other two behaviors. In (b) the behavior is shown, however 25 time points were interpolated. Consequently, quantitativ are much stronger — and the 2 impossible behaviors have been pruned. Table 1 intermediate stages in the simulation.

Variable→	Acceleration		Velocity		Height		Time		#
TIME→	153	T1	153	T2	153	T1	T1	T2	beh's
Stage↓									
(a) Phase I		[−9.83, 0)		(−∞, 0)		(0, ∞)	[305, ∞)	[305, ∞)	3
(b) 1 interp.	[−9.16, −8.44]	[−9.16, 0)	[1496, 2009]	,,	[229, 505]	[229, ∞)	[316, ∞)	[316, ∞)	1
(c) 4 interp.	[−8.99, −8.57]	[−8.77, 0)	[1535, 1948]	,,	[289, 452]	[373, ∞)	[326, ∞)	[326, ∞)	1
(d) TIS	,,	,,	,,	,,	,,	,,	,,	[519, ∞)	
(e) 7 interp.	[−8.91, −8.64]	[−8.65, 0)	[1558, 1919]	,,	[319, 424]	[422, ∞)	[331, ∞)	[51	
(f) Beh. split	,,	[−8.65, −.00052]	,,	,,	,,	[422, 866624]	[331		
(g) 8 interp.	,,	[−8.63, −7.98]	,,	(−∞, −1044]	,,	[428, 69			
(h) 25 interp.	[−8.87, −8.68]	[−8.56, −8.06]	[1570, 1905]	[−5482, −1819]	[334, 409]	[4			
(i) 50 interp.	[−8.87, −8.69]	[−8.53, −8.10]	[1572, 1902]	[−4653, −2137]	[3				

Table 1: The returning rocket simulation at vario
variables are each shown at TIME=153 (the
algorithm), and either T1 when the
on the way down. Each techni
interval results get nar
the text.)

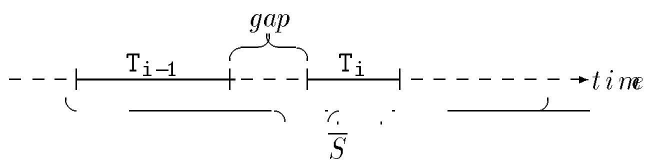


Figure 7: T_{i-1} and T_i are time *points*, but their values are known only to within intervals, in
by solid line segments. Between them is a gap. T_{i-1} and T_i are the endpoints of a tim
size is in $[w(gap), \overline{S}]$, where $w(gap)$ is the width of the gap. $\overline{S}$ is the maximum pos
from T_{i-1} to T_i.

3 Detailed Example: a Nonlinear Second-Order Roc

We now step through an example requiring step size refinement and the aux
offers. Consider a rocket in a gravitational field which decreases with th
second order and nonlinear, and hence makes a useful demon
model appears in Figure 8. The simulation for this ex
scribing known quantitative data about the Earth
than the escape velocity of $11,000 \frac{m}{s}$ so
To direct Q3's operation, we s

Goal: *"Prune as many beh*
havior(s)."

To minimize the potential
subgoal to pursue, give

Subgoal 1:

Phase I of a
bounds o
t

```
(define-QDE escape-velocity
  (text "Gravity decreases with height as r''=-GM/r^2")
  ; Define model variables and their qualitative values.
  (quantity-spaces
    (r       (0    sea-level inf)  "meters from Earth's core")
    (r^2     (0    inf         )  "distance squared"        )
    (h       (0    inf         )  "meters above surface"    )
    (km      (0    inf         )  "kilometers above surface")
    (surface (0    s*          )  "depth of Earth"          )
    (dr/dt   (minf 0 r*     inf)  "velocity, m/s"           )
    (d2r/dt2 (minf 0        inf)  "acceleration, m/s^2"     )
    (G       (0    G*          )  "Gravitational constant G")
    (Earth-M (0    M*          )  "Mass of Earth M"         )
    (K       (0    K*          )  "K (=G*M)"                )
    (-K      (-K*  0           )  "-K"                      )
    (=1000   (0    1000        )  "Thousand"                ))
  ; The model defines these constraint templates
  (constraints
    ((mult   km      =1000   h ))
    ((add    surface h       r  ) (s* 0 sea-level))
    ((mult   r       r       r^2)               )
    ((mult   G       Earth-M K  ) (g* m* k*)    )
    ((minus  k       -k         ) (k* -k*)      )
    ((mult   d2r/dt2 r^2    -K  )               )
    ((d/dt   r       dr/dt      ))
    ((d/dt   dr/dt   d2r/dt2    ))
    ((constant surface))
    ((constant G))
    ((constant Earth-M))
    ((constant k))
    ((constant -k))
    ((constant =1000))) )
```

Figure 8: **Qualitative model of a second order nonlinear system.** A list of quantity-spaces describes the qualitative values the various model variables can have, and a list of constraints describes the relationships among those model variables. This model describes an object in free fall in the Earth's gravitational field, such as a rocket or other projectile fired upward or an o falling downward. Gravity decreases with distance according to the standard nonl order differential equation

$$\frac{d^2r}{dt^2}=\frac{-GM}{r^2}.$$

```
(def-quantitative-info
  (name initial-velocity-about-3000)
  (quantitative-initializations
    ;gravitational constant
    (G       (G*         (6.67e-11     6.67e-11)))
    ;Earth's mass
    (Earth-M (M*         (5.98e24      5.98e24 )))
    ;radius of Earth
    (r       (sea-level  (6.37e6       6.37e6  )))
    ;Initial condition, less than escape velocity
    (dr/dt   (r*         (3000         3300    ))))
  (envelopes ()))
```

Figure 9: Quantitative data describing known facts about the Earth, as well as the incompletely specified initial velocity dr/dt of a rocket (Figure 8) fired upward from the Earth's surface.

each behavior. For the return behavior this was at time 153. For the escape behaviors, whi
T1=∞, it occurred at time 1000 (Section 4.2.1). Constraint propagation on the resul
network for each behavior pruned the escape behaviors and improved the ch
return behavior somewhat. The pruning of an escape behavior is des
improved characterization of the return behavior was described
Subgoal 1 has been fully satisfied but the overall G
still know little about how high the rock
narrow existing intervals, and inf
in the return behavior. T

Subgoal 2

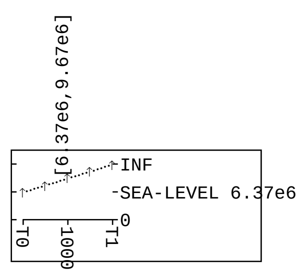
and

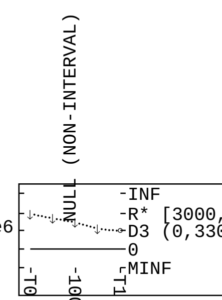
Subgo

Step

CONSTRAINT	INFERENCE	REASON
Initial Conditions	R_{T0} = SEA-LEVEL = 6.37e6 meters (i)	Given
	$(DR/DT)_{T0} \in [3000, 3300]$ m/s (ii)	
Previously Inferred	-K* = −3.99e14 (iii)	From G* and M* in Ph
	$(D2R/DT2)_{T0} = -9.83$ m/s^2 (iv)	From $(R\hat{}2)_{T0}$ and -K i
MEAN VALUE	$RATE(T0) \cup RATE(1000) = (-\infty, 3300]$; (v)	Qualitative behavior h decreasing; use that
RATE variable: DR/DT (velocity, m/s upward)	Decrease $\overline{R_{1000}}$; $R_{1000} \in (-\infty, 9.67e6]$	Solve equation (4) for $LEVEL(T_n)$ usin (i), (ii), and (v).
LEVEL variable: R (radius, meters from the Earth's center)	Increase $\underline{(DR/DT)_{1000}}$; $(DR/DT)_{1000} \in (0, \infty)$ (vi)	Qualitative be $R_{1000} > R_{T0}$, implies tha
TIME T_{n-1} = T0 = 0, T_n = 1000	Increase $\underline{R_{1000}}$; $R_{1000} \in (6.37e6, 9.67e6]$ (vii)	Solve equa $LEVEL(T_n)$ (i), (ii), and
MULTIPLICATION R×R = R^2, so $R_{1000} \times R_{1000} = (R\hat{}2)_{1000}$	Increase $\underline{(R\hat{}2)_{1000}}$; Decrease $\overline{(R\hat{}2)_{1000}}$; $(R\hat{}2)_{1000} \in [4.06e13, 9.35e13]$ (viii)	Squ
MULTIPLICATION (D2R/DT2) × (R^2) = -K, so $(D2R/DT2)_{1000} \times (R\hat{}2)_{1000}$ = $-K_{1000}$ = -K*	Increase $\underline{(D2R/DT2)_{1000}}$; Decrease $\overline{(D2R/DT2)_{1000}}$; $(D2R/DT2)_{1000} \in [-9.83, -4.27]$	
MEAN VALUE RATE variable: D2R/DT2 (acceleration of gravity, m/s^2) LEVEL variable: DR/DT *TIME* T_{n-1} = T0 = 0, T_n = 1000	Prune behavior; $DR/DT)_{1000} \in (0, \infty)$ and $(DR/DT)_{1000} \in [-6830, -965.5]$ have a null intersection; inconsistency detected.	

(a) Trace ↗





(b) Plot ↗

Radius = r(t) Velocity = dr/d

Table 2: (a) Excerpt of a trace showing how constrai
rocket, after a state was interpolated at time
(b) A plot for a pruned escape behavi

because behavior splitting creates new branches in the behavior tree and hence can lead to high computational complexity in subsequent simulation refinement. Thus, target interval splittin ("TIS") is used next, to try raising $\underline{\texttt{T2}}$ and lowering $\overline{\texttt{T1}}$.

Starting with the knowledge that $\texttt{T2} \in [326, \infty]$, Q3's implementation of target inte assumed $\texttt{T2} \in [326, 434]$, let the simulation settle via constraing propagation a that settling led to an inconsistency (Table 2 exemplifies detecti $\texttt{T2} \notin [326, 434]$, so $[326, 434]$ was trimmed from the interva successfully ruling out $[326, 434]$, target interval $[326, 651]$. Subsequent to ruling out out the adjacent interval $[482, 536]$, s approaching point values in the limit if the model is specified with real valued initial conditions and model parameters. When the model is specified imprecisely with one or more intervals we are interested in *stability*, which intuitively means that if system specifications are wea widths of result intervals will be wider but only to a limited degree. We first c followed by convergence, stability and finally termination for step si

4.1 Correctness

Numerical methods estimate answers, and interval methods bound the that the bounds safely contain the space of possible answers (e may also include extraneous values, which may occur for

- *Excess width.* This is a well-known problem i 1979; see also e.g. Abelson & Sussman The simplest such expression is (X give a weaker answer. For exam $X - X = [1, 2] - [1, 2] = [$ containing subtractio once. Eliminati either

4.2 Convergence

For numerical simulation, convergence means improving point predictions all the way to full accuracy (Gear 1971). For interval simulations, convergence means narrowing interval enclosures all the way to correct point predictions (Eijgenraam 1981 p. 57; Moore 1979 pp. 96–97; Lohner 1987 p. 261). Both senses apply in the limit as the step size of the simulation approaches zero.

As the step size decreases, the total number of steps increases. The computatio
of simulations containing a large number of steps, together with round-off er
point arithmetic or the compensating extra width added intention
metic, restricts convergence in practice. Nevertheless,
simulation algorithms.

Our analysis builds on traditional analys
as Euler's method (Gear 1971; also se
(Appendix B) states:

Let $\mathbf{Y}' = \mathbf{F}(\mathbf{Y})$ *be a system of*
valued functions of $\mathbf{Y}$. *We con*
component $Y_{(j)}$ *of vector* $\mathbf{Y}$, $Y_{(j)}$
$[lo, hi]$, *and that each* F_i *in vector* $\mathbf{F}$
$f_i(y)$.[7]

Let h *be the maximum step size,*
estimate of $\mathbf{Y}$ *at interpolated tim*
represent the amount of uncertainty
such that

Given precise initial conditions
that $\|Y_n\| \to 0$ as $h \to 0$. This c
can be reduced arbitrarily c
starting at time t
propagation c
be c

particular system suffers from excess width. For example, as Davis (1987) points out,

$$x \in [1,2] \quad implies \quad \frac{x+1}{x} \in [\frac{3}{2}, 2]$$

but straightforward calculation (e.g. by hand or in Q3), gives

$$\frac{x+1}{x} \in \frac{[1,2]+1}{[1,2]} = \frac{[2,3]}{[1,2]} = [\frac{2}{2}, \frac{3}{1}] = [1,3].$$

Thus this example demonstrates convergence despite excess width.

4.2.1 The infinitesimal step size assumption

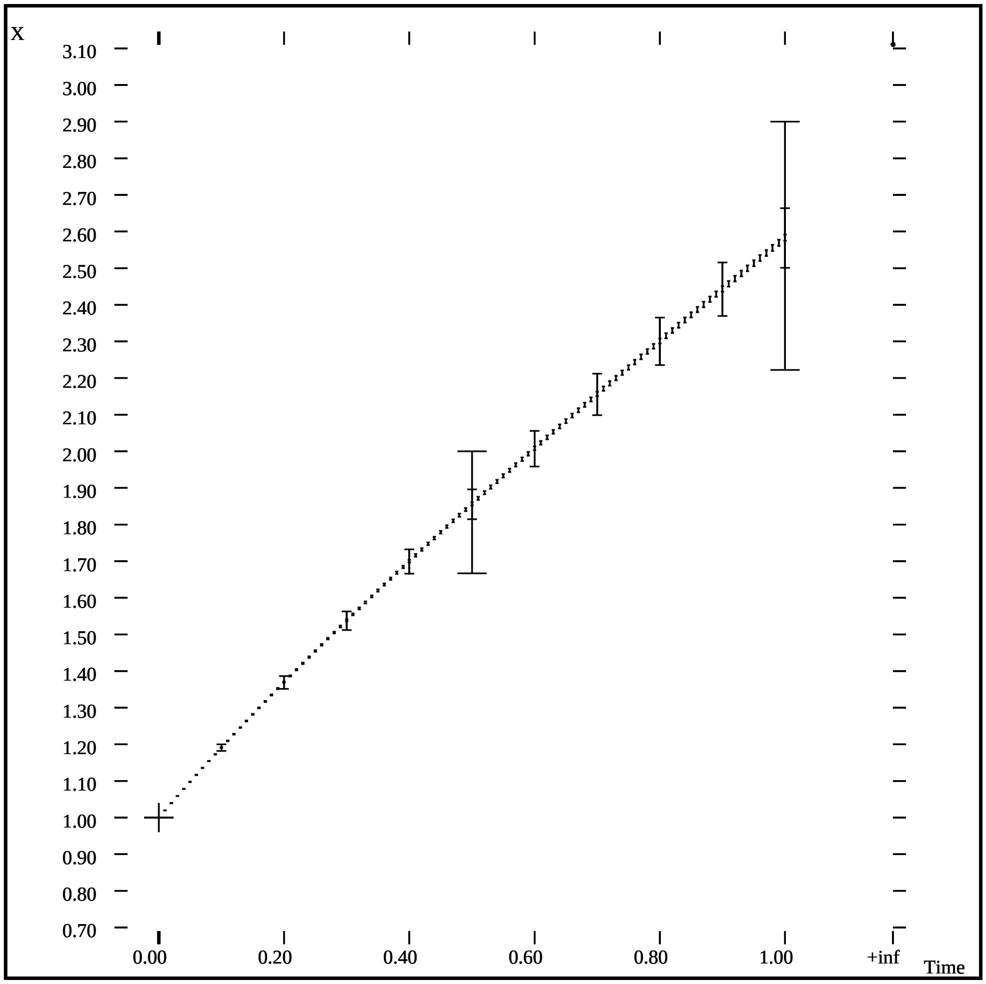
Convergence as a theoretical property (both in numerical simulation and in the present c
assumes that the step size can be made infinitesimally small. We discuss this issue in
below.

- If interpolation of each new time point can be done so as to reduce the si
S in the region in which convergence is desired, then continued
strictly monotonic decrease in the maximum step size in

Example: if the region of convergence is [0,1] su
and 0.875 would not be allowed because a
before the gap (0.75,1) if a strictly

- The decrease in maximum ste
strictly monotonic, but
two smaller ste
predefined co

Example: if
0.1



$$\frac{dx}{dt} = \frac{x+1}{x},\ x(0) = 1$$

Figure 10: Example of convergence even though the interval calculations produce excess width. A simulation for $\frac{dx}{dt} = \frac{x+1}{x}$ reveals a slightly concave down curve. Before step size refinement there are time points at 0 and ∞. After refining the simulation by interpolating two new states at tim values $t = 0.50$ and $t = 1.00$, uncertainty in x increases rapidly, as shown by the two tall in delimiters at $t = 0.50$ and $t = 1.00$. After refinement with ten interpolations, the t significantly more constrained, as shown by the ten interval delimiters of in times 0.10, 0.20, etc. Refinement with 100 interpolations leads to muc the 100 much shorter interval delimiters.

While convergence is universally recognized as an important theoretical property of simulation
methods for continuous systems, it should be noted that pragmatically oriented uses of time poi
interpolation have not had convergence as a goal (Dvorak 1992; Kay 1996; this paper Se
and especially 5.3.2). Pragmatically oriented work shows that even one interpolat
significantly improved quantitative bounds on model trajectories (Berleant
detailed example).

43 Stability

In numerical simulation stability is, intuitively, the desirable ch
starting values by a fixed amount produces a bounded ch
a well-posed problem and sufficiently small step siz
Gear (1971 p. 56) defines stability more fo

$$\| \mathbf{y}_n - \tilde{\mathbf{y}}_n \|$$

where $\mathbf{y}_0$ and $\tilde{\mathbf{y}}_0$ are two sets of initial con
numerical simulation after n steps wit
vector generalization of absol
equations containi
some posi
We ad

4.3.1 Gap existence and creation

While step size refinement is stable, convergent, and correct, it can only run within a gap. The most common and important case is a gap starting at T0 $\in [0,0]$. In particular:

- When the behavior has two qualitative time points T0=0 and T1=∞ the gap between T0 and T1 includes all positive finite values, allowing states to be interpolated at arbitrary time step size refinement is unimpeded.
- When $0 <$ T1 $< \infty$, the first gap is the open interval (0, T1), and step size refi unimpeded for time values in that interval. T1 may also increase as the sim more refined, increasing the size of the gap. (This occurred in Table

While often the requisite gaps will exist prior to step size re intervals in Phase I of the progressive simulation refinement may not, due to weak initial conditions. Q3 provid

- Use *target interval splitting.* See Appen
- Use *behavior splitting* to force a p
- Use another time step that
- Interpolate using a gap

Example: step size r in Figure 11.

4.3.2 Termination

Constraint propagation i have a finite numb or other labe termina

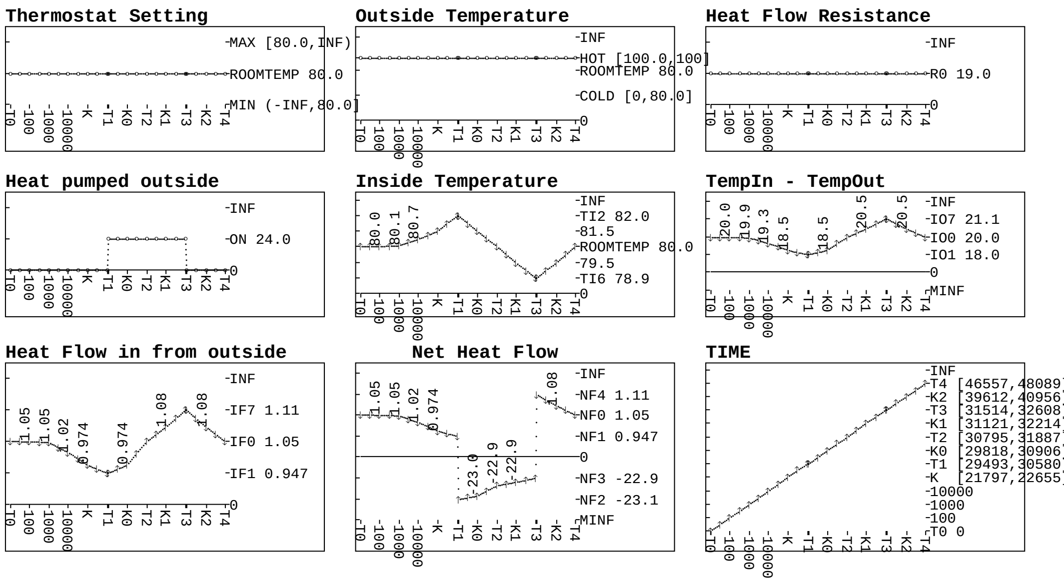


Figure 11: Piecewise continuous simulation of an air conditioned dwelling. The time points in this simulation come from three sources: (1) qualitative simulation, which created time points T0, T T2, T3 and T4; (2) interpolations in the gap between T0 and T1, which created time poin 1000, and 10000; and (3) interpolations in gaps of model variable Inside Tempera created time points K, K0, K1 and K2 at temperatures 79.5 and 81.5. Disconti some of the plots are caused by transitions between models.

5.1 Improved predictions

By making quantitative inferences, semi-quantitative simulation can often prune qualitative behaviors that are plausible from a purely qualitative standpoint. A behavior is pruned when quantitative
inference reveals that no interval is possible for some model variable at some time point (as we s
in Table 2). Dalle Molle (1989) and Dalle Molle and Edgar (1991) used phase I of Q3 (Q2)
purpose with two models of chemical engineering systems, the relatively simple but
of two parallel first-order chemical processes, and the less simple adiaba
reactor.

Farquhar and Brajnik (1994) used phase I of Q3 in a syste
Physics Compiler"). They generated semi-quantitative m
were able to model and simulate a real hydroelectr
levels for different water control scenarios.

5.2 Diagnosis

Semi-quantitative simulation can help diagnos
Models for which all behaviors are i
one remaining fault model
version (Dvorak 1992

5.3 Measuremen

The concept of interpolati
measurement parti
power of th

5.3.1

Suppose t
t=3375

Variable→	Velocity			Height		
Time point→	400	3000	T1	400	3000	T1
No measurement	[6770, 18867]	[906, 17870]	[0, 0]	[2950, 7862]	[10706, 55171]	[10924, ∞)
Weak measurement: Height ∈ [12000, 12500] at time=3375	[6770, 18463]	[906, 14295]	[0, 0]	[2950, 4558]	[10706, 12314]	[12025, ∞)
Strong measurement: Height = 12000 at time=3375	[6770, 18293]	[906, 13844]	[0, 0]	[2950, 4058]	[10706, 11814]	[12025, ∞)

Variable→	Acceleration		
Time point→	400	3000	T1
No measurement	[−4.59, −1.97]	[−1.37, −0.105]	[−1.34, 0)
Weak measurement: Height ∈ [12000, 12500] at time=3375	[−4.59, −3.34]	[−1.37, −1.14]	[−1.18, 0)
Strong measurement: Height = 12000 at time=3375	[−4.59, −3.67]	[−1.37, −1.2]	[−1.18, 0)

Table 3: Effects of different measurement strengths on predictions for Velocity, Height, and A
eration of the rocket, at time points 400, 3000, and T1. The intervals for the "no r
condition are the same as in Figure 5. The effects of interpolating a state with a
measurement condition are shown in the middle rows. A strong measureme
the last rows. Notice how predicted intervals tend to narrow as str
introduce stronger quantitative information into the simulat

The interpolation method of measurement interpretation contrasts with DeCoste's DATMI system
(1991) and its precursor ATMI (Forbus 1986). A significant difference is that DATMI abstracts
measurements into qualitative categories before using them, whereas MIMIC and Q3 use the ac
measured quantitative information. Hence DATMI loses quantitative information retai
by MIMIC and Q3.

DATMI is intended for handling large numbers of measurements. The unmodifie
unwieldy for large numbers of measurements, but can be modified to circumve
by propagating forward but not backward in time, and propagating forwa
This was the approach taken by MIMIC.

5.4 Bounding the probabilities of qualitative behaviors

Qualitative simulation alone can find all possible behaviors of a system but not their
Adding quantitative information can help. Q3 was part of a system that i
the qualitative behaviors of a fault tolerant system (Berleant
functions (pdfs) were used instead of intervals to d
informative than intervals. An interval repres
zero beyond the interval endpoints,
The pdfs were first discre
interval. Thus problem
intervals and sol
the di

NSIM (Kay and Kuipers 1993) and SQSIM (Kay 1996) were developed in part to alleviate the wide bounds that Q3's predecessor Q2 often infers. While NSIM sometimes provides better bounds than Q2 (Kay and Kuipers 1993; Kuipers 1994), sometimes NSIM's results are poorer than Q2's result which led to SQSIM which combines features of both NSIM and Q2. Kay (1996) desc SQSIM in detail but no comparison of its inferential ability to that of Q3 exists.

6.2 Numerical work

Forbus & Falkenhainer (1990, 1992) combined numerical and qualitative simulations i (SIMulator GENeration) system, building on qualitative process theory (Forbus plays notable advantages.

1. Use of qualitatively inferred model transitions (e.g. when v and boiling commences) enabling automating simulatio simulations.

2. Causal ordering applied to qualitative models

Limitations of SIMGEN include (1) the re the need for precise numerical informa approximate outputs and often While SIMGEN used (1991) used nume iors as s

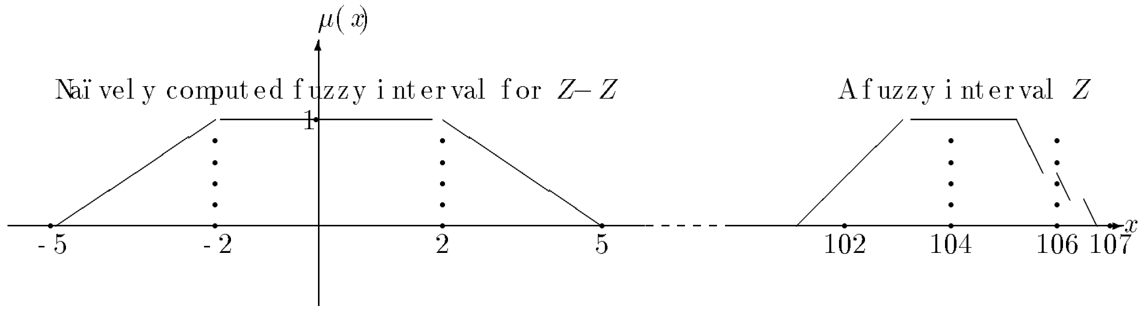


Figure 12: Fuzzy intervals. Sloping line segments indicate fuzzy regions. The lower the value of membership function $\mu(x)$, the less the degree of membership for x in the fuzzy interval.

6.3.1 As with standard intervals, operations on fuzzy intervals can produce excess width

Figure 12 contains a very simple example of how the excess width problem in calculations on
intervals has similar manifestations in calculations on fuzzy intervals. Values of x in t
terval $[104, 106]$ are full members of fuzzy interval Z, and those in the sloping a
sible members. Subtraction would give the region of full membership in the
$[104, 106] - [104, 106] = [-2, 2]$, the region of non-zero membership as $[102,$
and fuzzy edges of constant slope. However, Z is perfectly correla
has full membership at 0 and zero membership everywhere e
trivial, such situations can be arbitrarily complex
Considering $\mu(x)$ as an upper bound on t
addresses the membership over-estimati
results containing excess widt
Correlated fuzzy simulat
cost of assuming all
case of Mo
Fuzzy

- *From interval simulation:* the guarantee that the trajectory of any real system conforming to an incompletely specified model is enclosed by one of the predicted semi-quantitative behavior descriptions.

- *From interval simulation:* $h \rightarrow 0$ stability.

- *From interval simulation:* convergence as uncertainty in the quantitative specificat maximum step size, both approach zero.

- *From qualitative and interval representations:* the ability to express and r from partial knowledge.

The capabilities of Q3 rely mostly on the following.

- *Step size refinement*, for adaptive reduction in step size by in mediate time points into a predicted behavior.

- *Propagation of interval labels* in constraint networ

Examples of graphical output from Q3 were p involving the domains of prediction, diagn abilities of qualitative behavior The significance of Q3 t because Q3 demonst quantitative s men

Target Interval Splitting (TIS): Outline

GIVEN: • $Y = X^2 - X$ and
$X \in [0,1]$

THEREFORE: • $Y \in [-1,1]$ by constraint propagation (shown in this Figure).

OBJECTIVE: • Narrow Y (the target) further, by testing and ruling out pieces of its current interval as in Figure 14.

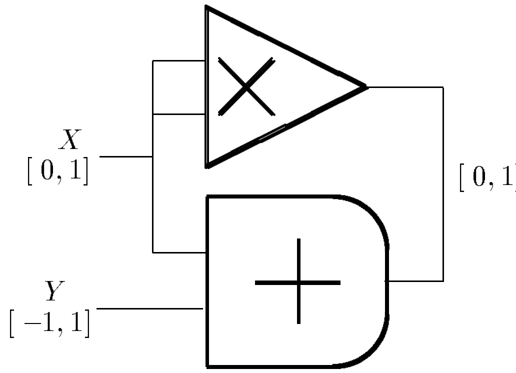


Figure 13: A constraint network for the equation $Y = X^2 - X$. Given $X \in [0,1]$, constraint propagation concludes $Y \in [-1,1]$. This conclusion is correct, but excessively weak, and is streng in Figure 14.

an equation a op $b = c$. Constraints over more than three quantities
in the mean value constraint, Sec
Transformatio

Iteration	Interval(s)	Reason
	TIS tests low bounds...	
1	$Y \in [-1, 1]$	constraint propagation
	$[-1, 0]$ $[0, 1]$	Split and test
2	$[-1, -0.5]$ $[-0.5, 1]$	Re-split and test
	X	Rule out
	$[-0.5, 1]$	Narrowed interval
3	$[-0.5, +0.25]$ $[+0.25, 1]$	Split and test
4	$[-0.5, -0.125]$ $[-0.125, 1]$	Re-split and test
5	$[-0.5, -0.3125]$ $[-0.3125, 1]$	Re-split and test
	X	Rule out
	$[-0.3125, 1]$	Narrowed interval
6	$[-0.3125, +0.3438]$ $[+0.3438, 1]$	Split and test
7	$[-0.3125, +0.0158]$ $[+0.0158, 1]$	Split and test
.	.	.
.	.	.
.	.	.
	$[-0.25 - \epsilon_1, 1]$	Conclude
	...then high bounds	
N	$[-0.25 - \epsilon_1, 1]$	Given
	$[-0.25 - \epsilon_1, +0.375 - \frac{\epsilon_1}{2}]$ $[+0.375 - \frac{\epsilon_1}{2}, 1]$	Split and test
.	.	.
.	.	.
.	.	.
	$[-0.25 - \epsilon_1, 0 + \epsilon_2]$	Conclude

Figure 14: **Target interval splitting narrows a target interval by ruling out piece**
The constraint network for $Y = X^2 - X$ was shown in Figure 13. Target interval split
tests the lower half of a target interval, $Y \in [-1, 1]$ in this example, by settin
propagating. If the network settles successfully (i.e. has a solution),
$[-1, -.5]$ in this case, the lower eighth if necessary, etc.
network has no solution. That sub-interval is
the lowest quarter, $Y \in [-1, -.5]$, wa
for the *highest* half, quart
above. For $Y = X$
reaching, $[-$
ϵ.

Proof: The proof has similarities with standard proofs of Euler's method (Gear 1
man 1976) and is also influenced by Moore (1979).
Y_n.

1. The inference method us

This and equation (12) justify

$$u(Y_n) \leq u(Y_{n-1}) + hLu(Y_{n-1} \cup (Y_{n-1} + hF(M))).$$

7. Since F is Lipschitz and a natural interval extension, $F(M)$ is bou
absolute value of an interval is the n

8.

Theorem 1 *Let* $\mathbf{Y}' = \mathbf{F}(\mathbf{Y})$ *be a system of first order differential equations, where* $\mathbf{F}$ *is a vector of interval valued functions of* $\mathbf{Y}$*. We consider some bounded subset* $[lo, hi]$ *of the reals such that for each component* $Y_{(j)}$ *of vector* $\mathbf{Y}$*,* $Y_{(j)}(t) \subseteq [lo, hi]$*. We assume that* $\mathbf{F}(\mathbf{Y})$ *is defined when each* $Y_{(j)} \subseteq [lo, hi]$*, and that each* F_i *in vector* $\mathbf{F}$ *is the natural interval extension of a real rational function* f_i*.*[7]

Let h *be the maximum step size, let* $\|\mathbf{Y}_{t=b}\|$ *represent the amount of uncertainty in the simulated estimate of* $\mathbf{Y}$ *at interpolated time point* $t = b$ *as measured by its vector norm*[8]*, and let* $\|\mathbf{Y}_0\|$ *represent the amount of uncertainty in the initial conditions. Then there are constants* K_1 *and* K_2 *such that*

$$\|\mathbf{Y}_{t=b}\| \leq K_1 \|\mathbf{Y}_0\| + K_2 h.$$

1. *Higher order systems:* The proof of Lemma 1 extends to higher order syste describe the higher order system as a syst

Each indivi

1. $E_{lowerEnvelope}$ and $E_{upperEnvelope}$ differ only in the values of some constants. Then, $G_{lowerEnvelope} \equiv$
$G_{upperEnvelope}$. Call this function G.

Consider each constant c_i whose value differs between $E_{lowerEnvelope}$
the lower of the values and $\overline{c_i}$ the higher one.
instead of $\underline{c_i}$ or $\overline{c_i}$. By

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