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Self-Calibrating Models for Dynamic Monitoring and Diagnosis.

NCC 2-760.

Final Report

covering the period
1 February 1992
to
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CASI

Self-Calibrating Models for Dynamic Monitoring and Diagnosis

The goal of this project is to develop and demonstrate a method for automatically building qualitative and semi-quantiative models of dynamic systems, and using them for monitoring and fault diagnosis. Our qualitative approach to modeling provides a guarantee of coverage while our semi-quantitative methods support convergence toward a numerical model as observations are accumulated. We have applied these methods to monitoring observation streams, and to the design and validation of non-linear control systems.

1 Research Results

We have made substantial progress in several areas: modeling of complex physical systems, semi-quantitative reasoning and monitoring, and tractable qualitative simulation. This work has resulted in five doctoral dissertations, and numerous publications in many different areas, including the definitive book on qualitative simulation. Most of these publications are available through our Web page: http://www.cs.utexas.edu/users/qr/.

1.1 Qualitative Reasoning Generally

Benjamin Kuipers has completed a book presenting the overall state of the QSIM approach to qualitative reasoning within a single coherent framework. By providing a common framework and notation, and an easily accessible source for the basic results, we hope that this book will help encourage and coordinate qualitative reasoning research at a number of different laboratories.

- B. J. Kuipers. 1994. *Qualitative Reasoning: Modeling and Simulation with Incomplete Knowledge.* Cambridge, MA: MIT Press. ISBN 0-262-11190-X. (pp. 414+xxvii.)

A number of other publications describe particular reasoning methods that exploit the qualitative representation, respond to controversies, or provide overviews of the closed and open problems in the field.

- B. Kuipers and J. Crawford. 1992. Guaranteed coverage vs intelligent sampling: a reply to Sacks and Doyle. *Computational Intelligence* **8**(2): 289-294.
- C. Chiu & B. J. Kuipers. 1992. Comparative analysis and qualitative integral representations. In Boi Faltings and Peter Struss (Eds.), *Recent Advances in Qualitative Physics*, MIT Press, 1992.
- P. Fouché & B. Kuipers. 1992. An assessment of current qualitative simulation techniques. In Boi Faltings and Peter Struss (Eds.), *Recent Advances in Qualitative Physics*, MIT Press, 1992.
- B. Kuipers. 1993. Self-calibrating models for dynamic monitoring and diagnosis. In *Proceedings of the Space Operations and Research Symposium (SOAR'93).* NASA Johnson Space Center, Houston, Texas, 3-5 August 1993.

- B. J. Kuipers. Reasoning with qualitative models. 1993. *Artificial Intelligence* **59**: 125-132.
- B. J. Kuipers. Qualitative simulation: then and now. 1993. *Artificial Intelligence* **59**: 133-140.

1.2 Model Building

The problem of automated model-building has been a major focus of our work, and we have addressed it from several different directions. Chapters 13 and 14 of Kuipers, *Qualitative Reasoning*, give an overview of our approaches to model-building.

Adam Farquhar completed his doctoral dissertation on QPC, a model compiler that composes qualitative models of complex physical systems, drawing upon domain theories represented by model fragment libraries. One major advance in QPC is that, like QSIM, it provides a coverage guarantee: if a physical situation can be modeled by the fragments in the domain library, the model-building algorithm will construct that model. Farquhar is now a research associate at the Stanford Knowledge Systems Lab where, among other responsibilities, he is extending QPC to a general-purpose compositional modeling language, CML.

- Adam Farquhar, *Automated Modeling of Physical Systems in the Presence of Incomplete Knowledge*. Doctoral dissertation, Department of Computer Sciences, University of Texas at Austin, Austin, Texas. December 1993.
- Adam Farquhar. 1994. A qualitative physics compiler. In *Proceedings of the National Conference on Artificial Intelligence (AAAI-94)*, AAAI/MIT Press, 1994.

During the summer of 1992, our group hosted Prof. Lyle Ungar and three of his students from the Chemical Engineering Department at the University of Pennsylvania, who are applying our tools to problems in chemical engineering.

QPC has been used (by C. Catino, a visiting chemical engineer from the University of Pennsylvania) to build a substantial domain theory for Hazard and Operability (HAZOP) studies of chemical plants. The domain library consists of 50+ model-fragments, and has been used to construct models as large as 280 variables and 340 constraints, making it one of the largest qualitative models ever built. Giorgio Brajnik, a visitor to our laboratory from Udine, Italy, has developed a semi-quantitative extension to QPC.

- Catherine A. Catino, *Automated Modeling of Chemical Plants with Application to Hazard and Operability Studies*. Doctoral dissertation, Department of Chemical Engineering, University of Pennsylvania, Philadelphia, Pennsylvania, 1993. (Professor Lyle H. Ungar, advisor.)
- Catherine A. Catino and Lyle H. Ungar. 1995. Model-based approach to automated hazard identification of chemical plants. *AIChE Journal* **41**(1): 97–109, January 1995.
- Adam Farquhar and Giorgio Brajnik. 1994. A semi-quantitative physics compiler. In *Working Papers of the International Workshop on Qualitative Reasoning (QR-94)*, 1994.

- Giorgio Brajnik. 1995. Introducing boundary conditions in semi-quantitative simulation. In *Ninth International Workshop on Qualitative Reasoning (QR-95)*, Amsterdam, May 1995.

QPC was used in the doctoral research of Jeff Rickel who developed methods to exploit knowledge of time-scale and natural system boundaries to formulate tractable models from a very large knowledge base to answer particular prediction questions. It was also used in the doctoral research of Raman Rajagopalan, who combined qualitative knowledge of spatial relations with dynamical systems to predict the behavior of physical systems involving magnetic fields, such a transformers, motors, and generators.

- Jeff Rickel and Bruce Porter. 1994. Automated modeling for answering prediction questions: selecting the time scale and system boundary. In *Proceedings of the National Conference on Artificial Intelligence (AAAI-94)*, AAAI/MIT Press, 1994.
- Jeff W. Rickel. 1995. *Automated modeling of complex systems to answer prediction questions.* Doctoral dissertation, Department of Computer Sciences, The University of Texas at Austin. (Professor Bruce Porter, advisor)
- Raman Rajagopalan. 1995. *Qualitative reasoning about dynamic change in the spatial properties of a physical system.* Doctoral dissertation, Department of Computer Sciences, The University of Texas at Austin. (Professor Benjamin Kuipers, advisor.)

We have constructed several qualitative models of the Space Shuttle Reaction Control System, to serve as a testbed for our methods. The first model was built by hand in QSIM by Herbert Kay.[1] Later, Takashi Watanabe, a visiting scholar from Nagoya, Japan, reimplemented our CC component-connection model-builder in the Algernon knowledge representation language that also underlies QPC. Using the new version of CC he built a component-connection model of the Reaction Control System.

- H. Kay. 1992. A qualitative model of the space shuttle reaction control system. University of Texas at Austin, Artificial Intelligence Laboratory Technical Report AI92-188.

[1]This model has subsequently been used by a number of other researchers, including the following.

- Deepak Kulkarni, Herbert Kay, and Peter Robinson. Diagnosis of Shuttle Reaction Control System (Extended Abstract). In *NASA Workshop on Monitoring and Diagnosis*, Pasadena, CA, January 1992.
- Richard S. Mallory, Bruce W. Porter, and Benjamin J. Kuipers. 1996. Comprehending complex behavior graphs through abstraction. In *Working Papers of the Tenth International Workshop on Qualitative Reasoning (QR-96)*, Fallen Leaf Lake, California.
- Siddarth Subramanian. Qualitative multiple-fault diagnosis of continuous dynamic systems using behavioral modes. Doctoral dissertation, Computer Science Department, University of Texas at Austin, December, 1995. Professor Ray Mooney, advisor.
- Siddarth Subramanian and Raymond J. Mooney. 1996. Qualitative multiple-fault diagnosis of continuous dynamic systems using behavioral modes. In *Proceedings of the National Conference on Artificial Intelligence (AAAI-96)*. AAAI/MIT Press, 1996.

- Takashi Watanabe and Benjamin Kuipers, *Component Connection Models of Reaction Control System.* Manuscript, January 1994.
- Takashi Watanabe, *CC-in-Algy: Algernon Based Component Connection Models.* Manuscript, 13 September 1993.

In addition to these methods, we have been exploring a method for learning qualitative models from observations of behavior. The MISQ algorithm essentially inverts the QSIM algorithm by using the behaviors to filter the set of all possible constraints that could appear in the model. The original idea was presented in 1992, and an extension to handle multiple operating regions was developed in 1994.

- Bradley L. Richards, Ina Kraan and Benjamin J. Kuipers. Automatic abduction of qualitative models. *Proceedings of the National Conference on Artificial Intelligence (AAAI-92)*, AAAI/MIT Press, 1992.
- S. Ramachandran, R. J. Mooney & B. J. Kuipers. 1994. Learning qualitative models for systems with multiple operating regions. In *Working Papers of the Eighth International Workshop on Qualitative Reasoning about Physical Systems (QR-94)*, Nara, Japan.

1.3 Semi-Quantitative Inference

Semi-quantitative reasoning annotates the qualitative behavior prediction with quantitative bounds on the values of qualitatively described terms: real bounded intervals around landmark values, and envelopes around monotonic functions. Dan Berleant and Ben Kuipers had developed Q2 and Q3, which defined the initial semi-quantitative representation, and showed that semi-quantitative reasoning could converge to real-valued predictions as uncertainty in the model reduces to zero.

Herbert Kay, collaborating with Kuipers and Ungar, has developed two major pieces of the semiquantitative reasoning puzzle. First, he created, implemented, and proved the soundness of the dynamic envelope method for predicting improved bounds on behavior trajectories, given bounds on landmark values and envelopes around monotonic functions. The dynamic envelope method complements Q2 and Q3 to provide much stronger bounds on the prediction than were previously possible. Second, in collaboration with Lyle Ungar of the University of Pennsylvania, he developed a method for acquiring bounds on incompletely known monotonic functions by analyzing streams of observations.

These methods make it possible to assimilate a stream of observations, reducing the uncertainty of a semi-quantitative model until it converges to a real-valued model, and thereby achieving the self-calibration portion of our project goal.

- D. Berleant & B. Kuipers. 1992. Combined qualitative and numerical simulation with Q3. In Boi Faltings and Peter Struss (Eds.), *Recent Advances in Qualitative Physics*, MIT Press, 1992.
- H. Kay and B. Kuipers. 1992. Numerical behavior envelopes for qualitative models. In *Working Papers of the Sixth International Workshop on Qualitative Reasoning about Physical Systems*, Edinburgh, Scotland.

- H. Kay & B. Kuipers. 1993. Numerical behavior envelopes for qualitative simulation. *Proceedings of the National Conference on Artificial Intelligence (AAAI-93)*, AAAI/MIT Press, 1993.
- H. Kay & L. H. Ungar. 1993. Deriving monotonic function envelopes from observations. *Proc. 7th Int. Workshop on Qualitative Reasoning About Physical Systems*, Orcas Island, Washington, pp. 117–123.
- Herbert Kay. 1996. SQsim: a simulator for imprecise ODE models. University of Texas Artificial Intelligence Laboratory TR AI96-247, March 1996.

1.4 Tractable Qualitative Simulation

The failure mode of a qualitative model is to predict vastly too many possible behaviors. One approach to making the set of predicted behaviors tractable is to use deeper mathematical knowledge about dynamical systems, and representations that make the relevant properties of the system explicit. Two examples of these are the analysis of energy (or equivalently, Lyapunov functions), and the use of the phase portrait as a representational tool.

Pierre Fouché developed an important method for making explicit the kinetic, potential, and total energy in certain systems, and testing their behaviors for consistency. Building on this and other methods, Wood Wai Lee completed a doctoral dissertation in which he shows that qualitative simulation can be used to construct qualitative phase portraits of non-trivial systems, inheriting the QSIM guarantees of complete coverage.

- Pierre Fouché & Benjamin Kuipers. 1992. Reasoning about energy in qualitative simulation. *IEEE Transactions on Systems, Man, and Cybernetics* **22**(1): 47-63.
- Wood Wai Lee. 1993. *A qualitative simulation based method to construct phase portraits.* Doctoral dissertation, Department of Computer Sciences, University of Texas at Austin, January 1993.
- W. W. Lee and B. Kuipers. 1993. A qualitative method to construct phase portraits. In *Working Papers of the Seventh International Workshop on Qualitative Reasoning about Physical Systems*, Orcas Island, Washington.
- W. W. Lee & B. Kuipers. 1993. A qualitative method to construct phase portraits. *Proceedings of the National Conference on Artificial Intelligence (AAAI-93)*, AAAI/MIT Press, 1993.

Daniel Clancy has been developing methods for abstracting the structure and behaviors of qualitative models to obtain tractable sets of predicted behaviors from realistically complex models. As the principal maintainer for the QSIM code, Clancy has been consulting with QSIM model-builders around the world in this research.

He has developed methods for isolating "chatter" (unconstrained branching) into loosely coupled "chatter boxes" in the behavior description; for recognizing and abstracting SISO (single-input-single-output) subgraphs produced by occurrence branching; and for recognizing weak causal interactions among components in the structural description, allowing the simulator to take a divide-and-conquer approach. Richard Mallory has developed a related method for abstracting models developed from a large knowledge base in biology.

Clancy, working with our Italian visitor, Giorgio Brajnik, has also been exploiting the use of temporal logic as a new way for the modeler to express constraints on qualitative behaviors. This makes it possible to include knowledge in the model that was previously inexpressible in the QDE constraint language. This work was inspired by our application of temporal logic model-checking for controller verification, but it treats temporal logic statements as inputs, rather than outputs, of the simulation process.

- D. J. Clancy and B. Kuipers. 1993. Behavioral abstraction for tractable simulation. *Proc. 7th Int. Workshop on Qualitative Reasoning About Physical Systems*, Orcas Island, Washington, pp. 57-64.
- D. Clancy and B. Kuipers. 1994. Model decomposition and simulation. In *Working Papers of the Eighth International Workshop on Qualitative Reasoning about Physical Systems (QR-94)*, Nara, Japan.
- Richard S. Mallory, Bruce W. Porter, and Benjamin J. Kuipers. 1996. Comprehending complex behavior graphs through abstraction. In *Working Papers of the Tenth International Workshop on Qualitative Reasoning (QR-96)*, Fallen Leaf Lake, California.
- Giorgio Brajnik and Daniel J. Clancy. 1996. Guiding and refining simulation using temporal logic. In *Proc. of the Third International Workshop on Temporal Representation and Reasoning (TIME'96)*, Key West, Florida, May 1996. IEEE Computer Society Press, pp. 144-151.
- Giorgio Brajnik and Daniel J. Clancy. 1996. Temporal constraints on trajectories in qualitative simulation. In *Working Papers of the Tenth International Workshop on Qualitative Reasoning (QR-96)*, Fallen Leaf Lake, California.
- Giorgio Brajnik and Daniel J. Clancy. 1996. Temporal constraints on trajectories in qualitative simulation. In *Proceedings of the National Conference on Artificial Intelligence (AAAI-96)*, AAAI/MIT Press, 1996.

1.5 Controller Verification

We also investigated the use of qualitative simulation as a method for verifying non-linear controllers, including controllers composed of several simple local controllers with overlapping operating regions.

We use temporal logic as a query language for the set of qualitative behavior predictions by interpreting the QSIM behavior tree as a temporal model structure, and using it to prove statements in temporal logic by model-checking. The temporal logic model-checking work was done in collaboration with Benjamin Shults.

The design and validation of non-linear controllers was done in collaboration with Karl Åström, and with colleagues from the University of Pennsylvania, Lyle Ungar and Warren Seider, and their student Evi Gazi. One further contribution from the Penn researchers was to extend this verification method to apply to the output of Monte-Carlo simulations.

Much of this research was funded separately by grants from NSF and EPRI, but it is reported here because the effort overlapped with, and is synergistic with, NASA-funded research.

- E. Gazi, H. Kay, B. J. Kuipers, W. D. Seider, L. H. Ungar. Controller verification using qualitative reasoning. (Extended abstract) American Institute of Chemical Engineers, 1993 meeting.

- B. J. Kuipers and B. Shults. 1994. Reasoning in logic about continuous systems. In J. Doyle, E. Sandewall, and P. Torasso, editors, *Principles of Knowledge Representation and Reasoning: Proceedings of the Fourth International Conference (KR-94)*, Morgan Kaufmann, San Mateo, CA.

- B. J. Kuipers and K. Åström. 1994. The composition and validation of heterogeneous control laws. *Automatica* **30**(2): 233–249.

- E. Gazi, L.H. Ungar, W.D. Seider and B.J. Kuipers. 1996. Automatic analysis of Monte-Carlo simulations of dynamic chemical plants. *Proceedings of ESCAPE-6*, (in press), 1996.

- E. Gazi, L.H. Ungar and B.J. Kuipers. 1996. Temporal logic for summarizing monte-carlo simulation: an application to controller verification. In R. Shoureshi (Ed.), *Intelligent Control*, IEEE, 1996, to appear.

- Benjamin Shults and Benjamin Kuipers. 1996. Qualitative simulation and temporal logic: proving properties of continuous systems. UT AI TR AI96-244. (Submitted for publication.)

2 Abstracts of Selected Papers

2.1 Qualitative Reasoning Generally

Qualitative Reasoning: Modeling and Simulation with Incomplete Knowledge

Benjamin Kuipers

Cambridge, MA: MIT Press, 1994.

Abstract

After fifteen years of work, the world of qualitative reasoning according to the QSIM viewpoint is now described in a single book.

Qualitative reasoning is one of the most vigorous areas in artificial intelligence. This book presents, within a conceptually unified theoretical framework, a body of methods that have been developed over the past fifteen years for building and simulating qualitative models of physical systems (bathtubs, tea kettles, automobiles, the physiology of the body, chemical processing plants, control systems, electrical circuits, and the like) where knowledge of that system is incomplete. The primary tool for this work is the author's QSIM algorithm which is discussed in detail.

Qualitative models are more able than traditional models to express states of incomplete knowledge about continuous mechanisms. Qualitative simulation guarantees to find all possible behaviors consistent with the knowledge in the model. This expressive power and coverage are important in problem-solving for diagnosis, design, monitoring, and explanation.

The framework is built around the QSIM algorithm for qualitative simulation, and the QSIM representation for qualitative differential equations, both of which are carefully grounded in continuous mathematics. Qualititative simulation draws on a wide range of mathematical methods to keep a complete set of predictions tractable, including the use of partial quantitative information. Compositional modeling and component-connection methods for building qualitative models are also discussed in detail.

Qualitative Reasoning is primarily intended for advanced students and researchers in AI or its applications. Scientists and engineers who have had a solid introduction to AI, however, will be able to use this book for self instruction in qualitative modeling and simulation methods.

2.2 Model Building

Automated Modeling of Physical Systems in the Presence of Incomplete Knowledge

Adam Farquhar
Doctoral dissertation
Department of Computer Sciences
University of Texas at Austin
August, 1993.
Advisor: Professor Benjamin Kuipers

Abstract

This dissertation presents an approach to automated reasoning about physical systems in the presence of *incomplete knowledge* which supports formal analysis, proof of guarantees, has been fully implemented, and applied to substantial domain modeling problems. Predicting and reasoning about the behavior of physical systems is a difficult and important task that is essential to everyday commonsense reasoning and to complex engineering tasks such as design, monitoring, control, or diagnosis.

A capability for automated modeling and simulation requires

- expressiveness to represent incomplete knowledge,
- algorithms to draw useful inferences about non-trivial systems, and
- precise semantics to support meaningful guarantees of correctness.

In order to clarify the structure of the knowledge required for reasoning about the behavior of physical systems, we distinguish between the *model building* task which builds a model to describe the system, and the *simulation* task which uses the model to generate a description of the possible behaviors of the system.

This dissertation describes QPC, an implemented approach to reasoning about physical systems that builds on the expressiveness of Qualitative Process Theory [Forbus, 1984] and the mathematical rigor of the QSIM qualitative simulation algorithm [Kuipers, 1986].

The semantics of QPC's modeling language are grounded in the mathematics of ordinary differential equations and their solutions. This formalization enables the statement and proof of QPC's correctness. If the domain theory is adequate and the initial description of the system is correct, then the actual behavior of the system must be in the set of possible behaviors QPC predicts.

QPC has been successfully applied to problems in Botany and complex examples drawn from Chemical Engineering, as well as numerous smaller problems. Experience has shown that the modeling language is expressive enough to describe complex domains and that the inference mechanism is powerful enough to predict the behavior of substantial systems.

A semi-quantitative physics compiler

Adam Farquhar and Giorgio Brajnik

Eighth International Workshop on Qualitative Reasoning (QR-94)
1994.

Abstract

Incomplete information is present in many engineering domains, hindering traditional and non-traditional simulation techniques. This paper describes SQPC (semi-quantitative physics compiler), an implemented approach to modelling and simulation that can predict the behavior of incompletely specified systems, such as those that arise in the water control domain. SQPC is the first system that unifies compositional modeling techniques with semi-quantitative representations. We describe SQPC's foundations, QSIM and QPC, and how it extends them. We demonstrate SQPC using an example from the water supply domain.

Introducing boundary conditions in semi-quantitative simulation.

Giorgio Brajnik

Ninth International Workshop on Qualitative Reasoning (QR-95),
1995.

Abstract

Boundary value problems specifying how external influences on dynamic systems vary over time greatly extend the scope of qualitative reasoning techniques, enabling them to achieve a much wider applicability. This paper discusses conceptual and practical aspects that underlie the problem of handling boundary conditions in SQPC, a sound program for modeling and simulating dynamic systems in the presence of incomplete knowledge. Issues concerning the ontology (actions vs. measurements), the temporal scale (instantaneous vs. extended changes), the impact of discontinuity on model structure and the consequences of incompleteness in predictions are discussed. On the basis of the experimentation done so far it is claimed that given the generality of the assumptions underlying the techniques presented in the paper, and given the relatively low computational cost that is often required to solve a boundary value problem, they are viable and can be utilized to widen the applicability spectrum of Qualitative Reasoning.

Automated Modeling of Chemical Plants
with Application to Hazard and Operability Studies

Catherine A. Catino
Doctoral dissertation
Department of Chemical Engineering
University of Pennsylvania
December 1993
Advisor: Professor Lyle H. Ungar

Abstract

When quantitative knowledge is incomplete or unavailable (e.g. during design), qualitative models can be used to describe the behavior of chemical plants. Qualitative models were developed for several different process units with controllers and recycle, including a nitric acid plant reactor unit, and simulated using QSIM. In general, such systems produce an infinite number of qualitative states. Two new modeling assumptions were introduced, perfect controllers which respond ideally to a disturbance and ignore dynamics in controller variables, and pseudo steady state which ignores transients in all variables. Redundant constraints, reformulated equations, and quantitative information were also used to reduce ambiguity.

A library of general physical and chemical phenomena such as reaction and heat flow was developed in the Qualitative Process Compiler (QPC) representation and used to automatically build qualitative models of chemical plants. The phenomenon definitions in the library specify the conditions required for the phenomena to occur and the equations they contribute to the model. Given a physical description of the equipment and components present, their connectivity and operating conditions, the automatic model builder identifies the phenomena whose preconditions are satisfied and builds a mathematical model consisting of the equations contributed by these active phenomena. Focusing techniques were used to ignore irrelevant aspects of behavior. A dynamic condenser model was automatically generated illustrating QPC's ability to create a new model when a new phase exists.

Based on the ability to automatically build and simulate qualitative process models, a prototype hazard identification system, Qualitative Hazard Identifier (QHI), was developed which works by exhaustively positing possible faults, simulating them, and checking for hazards. A library of general faults such as leaks, broken filters, blocked pipes, and controller failures is matched against the physical description of the plant to determine all specific instances of faults that can occur in the plant. Faults may perturb variables in the original design model, or may require building a new model. Hazards including over-pressure, over-temperature, controller saturation, and explosion were identified in the reactor section of a nitric acid plant using QHI.

Automated Modeling of Complex Systems to Answer Prediction Questions

Jeff Rickel
Doctoral dissertation
Department of Computer Sciences
University of Texas at Austin
1995.
Advisor: Professor Bruce Porter

Abstract

The ability to answer prediction questions is crucial in science and engineering. A prediction question describes a physical system under hypothetical conditions and asks for the resulting behavior of specified variables. Prediction questions are typically answered by analyzing (e.g., simulating) a mathematical model of the physical system. To provide an adequate answer to

a question, a model must be sufficiently accurate. However, the model must also be as simple as possible to ensure tractable analysis and comprehensible results. Ensuring a simple yet adequate model is especially difficult for complex systems, which include many phenomena that can be described at many levels of detail. While tools exist for analysis, modeling is a creative, time-consuming task performed by humans.

We have designed algorithms for automatically constructing models to answer prediction questions, implemented them in a program called TRIPEL, and evaluated them in the domain of plant physiology. Given a prediction question and domain knowledge, TRIPEL builds the simplest differential-equation model that can adequately answer it and automatically passes the model to a simulator to generate the desired predictions. TRIPEL uses knowledge of the time scales on which processes operate to identify and ignore insignificant phenomena and choose quasi-static representations of fast phenomena. It also uses novel criteria and methods to choose a suitable system boundary, separating relevant subsystems from those that can be ignored. Finally, it includes a novel algorithm for efficiently searching through alternative levels of detail in a vast space of possible models. TRIPEL successfully answered plant physiology questions using a large, multipurpose, botany knowledge base (covering 300 processes and 700 plant properties) independently developed by a domain expert. Because its methods are domain-independent, TRIPEL should be equally useful in many areas of science and engineering.

Automated Modeling for Answering Prediction Questions: Selecting the Time Scale and System Boundary

Jeff Rickel and Bruce Porter

AAAI-94
AAAI/MIT Press, Cambridge, MA, 1994.

Abstract

The ability to answer prediction questions is crucial to reasoning about physical systems. A prediction question poses a hypothetical scenario and asks for the resulting behavior of variables of interest. Prediction questions can be answered by simulating a model of the scenario. An appropriate system boundary, which separates aspects of the scenario that must be modeled from those that can be ignored, is critical to achieving a simple yet adequate model. This paper presents an efficient algorithm for system boundary selection, it shows the important role played by the model's time scale, and it provides a separate algorithm for selecting this time scale. Both algorithms have been implemented in a compositional modeling program called TRIPEL and evaluated in the plant physiology domain.

Qualitative reasoning about dynamic change in the spatial properties of a physical system.

Raman Rajagopalan.

Doctoral dissertation
Department of Computer Sciences
The University of Texas at Austin
1995.
Advisor: Professor Benjamin Kuipers

Abstract

Spatial reasoning is an essential part of human interaction with the physical world. Of the many models that have been developed to support automated spatial reasoning, most rely on numerical descriptions of a spatial scene. This dissertation addresses problems where only qualitative descriptions of a spatial scene are available, such as natural language understanding, qualitative design, and physics problem-solving.

We provide the first set of solutions, given only a qualitative description of a spatial scene, for reasoning about dynamic change in both the spatial and non-spatial properties of a physical system. We use diagrams to compactly input the spatial scene for a problem, and text to describe any non-spatial properties. To match diagram and text objects so their descriptions can be integrated, we have developed a method for describing the conceptual class of objects directly in diagrams. Then, diagram and text objects can be matched based on their conceptual class.

The given problem is solved through qualitative simulation, and all spatial reasoning is done with respect to an extrinsic Cartesian coordinate system. We model the relative positions of objects through inequality constraints on the coordinates of the points of interest. Changes due to translational motion are detected by noting changes in the truth values of inequality constraints. We model the orientation of an object through knowledge of its extremal points and its qualitative angle of rotation with respect to each coordinate axis. This model has been used to reason qualitatively about the effects of rotational motion, such as changes in the area projected by one object onto another.

We have implemented our spatial representation as production rules and as model fragments in the QPC qualitative modeling system. The former has been used for solving static-world problems such as understanding descriptions of an urban scene. The latter has been used to reason about situations where changes in spatial properties play a critical role, such as the operation of transformers, oscillators, generators, and motors. To support dynamic spatial reasoning, we have expanded the modeling capabilities of QPC to include methods for modeling piecewise-continuous variables, non-permanent objects, and variables with circular quantity spaces.

Component Connection Models of the Reaction Control System

Takashi Watanabe and Benjamin Kuipers
Department of Computer Sciences
University of Texas at Austin
Manuscript, January 1994.

Abstract

Many of engineering devices consists of components, and component centered modeling presents us a straight way to build global systems of the devices. This modeling is also expected to give representations with minimum redundancy, which are easy to rearrange and are easy to understand for human. We demonstrate component connection models in QSIM and shows its utility.

While we note that the original component connection model (CC) on QSIM has smart ideas, we developed a new model builder which inherits the concepts from CC and has extended facilities in order to perform qualitative and semiquantitative simulations on QSIM. The new model builder (CC-in-Algy) is based on Algernon, and almost all the modeling data are held in frames and these data are accessed by inference rules which create QDE definitions. Each component has local constraints in it, and connections of components produces additional constraints between terminals. In order to obtain tractable behaviors, it is, however, sometimes required to use constraints among variables in different components, and it is also necessary to inherit sufficient data from predecessor states at region transitions. CC-in-Algy enables us to represent both of them.

As an application of component connections of CC-in-Algy, this paper describes the simulation of the space shuttle reaction control system (RCS). Tanks, regulators, pipes and thrusters constitute RCS, and each of them or a group of some of them makes a component which is used to build a global model of RCS.

CC-in-Algy: Algernon Based Component Connection Models

Takashi Watanabe
Department of Computer Sciences
University of Texas at Austin
Manuscript, September 1993.

Abstract

CC-in-Algy is an Algernon based QSIM model builder which interprets components and their connections, and creates global QDE definitions. It follows the concepts of the original CC [Franke and Dvorak 90], and gives a platform of component-connection paradigm. While the original CC has some functions (e.g. define-component-interface, define-component-implementation, define-quantity-space) in order to define components, CC-in-Algy offers only one function define-component). The prototype of the function define-component which consists of some of original CC definition functions are presented and demonstrated by Kuipers [Kuipers 92]. The function define-component in CC-in-Algy gives complete compatibility with the original definition and some extensions used for semiquantitative simulations and simulations with hierarchical quantity spaces. We can, therefore, see that CC-in-Algy presents compact representations of component definitions in comparison with the original CC.

The main part of CC-in-Algy is written in a frame based logical programming language Algernon [Kuipers and Crawford 93]. All the component data including variables, connections, terminals, connections and m-envelopes are represented in frames of Algernon, and these data

are processed by forward and backward inference rules. This is expected to give an easy way for the maintenance of CC-in-Algy.

Section 2 describes the component definition macro and some features of CC-in-Algy, Section 3 gives explanations about implementation and executions of CC-in-Algy, Section 4 describes the internal processing, and Section 5 shows some utility functions and the extension of domains.

It is highly recommended to refer to the manual of the original CC in order to know the background and concepts of component connections.

2.3 Semi-Quantitative Inference

Numerical Behavior Envelopes for Qualitative Simulation

Herbert Kay and Benjamin Kuipers

AAAI-93
AAAI/MIT Press, Cambridge, MA, 1993.

Abstract

Semiquantitative models combine both qualitative and quantitative knowledge within a single semiquantitative qualitative differential equation (SQDE) representation. With current simulation methods, the quantitative knowledge is not exploited as fully as possible. This paper describes *dynamic envelopes* – a method to exploit quantitative knowledge more fully by deriving and numerically simulating an *extremal system* whose solution is guaranteed to bound all solutions of the SQDE. It is shown that such systems can be determined automatically given the SQDE and an initial condition. As model precision increases, the dynamic envelope bounds become more precise than those derived by other semiquantitative inference methods. We demonstrate the utility of our method by showing how it improves the dynamic monitoring and diagnosis of a vacuum pumpdown system.

Deriving Monotonic Function Envelopes from Observations

Herbert Kay and Lyle H. Ungar

Seventh International Workshop on Qualitative Reasoning (QR-93)
1993

Abstract

Much work in qualitative physics involves constructing models of physical systems using functional descriptions such as "flow monotonically increases with pressure." Semiquantitative methods improve model precision by adding numerical envelopes to these monotonic functions. Ad hoc methods are normally used to determine these envelopes. This paper describes a systematic method for computing a bounding envelope of a multivariate monotonic function given a stream of data. The derived envelope is computed by determining a simultaneous confidence band for a special neural network which is guaranteed to produce only monotonic functions. By composing these envelopes, more complex systems can be simulated using semiquantitative methods.

SQsim: a simulator for imprecise ODE models

Herbert Kay

University of Texas Artificial Intelligence Laboratory TR AI96-247
March 1996.

This article describes a method for representing and simulating Ordinary Differential Equation (ODE) systems which are imprecise – that is, where the ODE model contains both parametric and functional uncertainty. Such models, while useful in engineering contexts, are not used in practice because they require either special structures which limit the describable uncertainty or produce predictions which are extremely weak. This article describes SQsim (for SemiQuantitative SIMulator), a system which provides a general language for representing and reasoning about many common types of engineering uncertainty. By defining the model both qualitatively and quantitatively and by using a simulation method that combines inferences across the qualitative-to-quantitative spectrum, SQsim produces predictions that maintain a precision consistent with the model imprecision.

2.4 Tractable Qualitative Reasoning

A Qualitative Simulation Based Method To Construct Phase Portraits

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January 1993.
AI 93-194

We have designed a qualitative simulation based method to construct phase portraits for a significant class of systems of two first order autonomous differential equations. It is intended as a step toward automated understanding of continuous physical systems. Differential equation models are powerful tools for reasoning about physical systems, but they typically require precise information about systems. Recently developed methods for qualitative simulation make it possible to predict all possible behaviors consistent with a state of incomplete, qualitative knowledge of the world, expressed as a qualitative differential equation (QDE). However, qualitative simulation can fail due to intractable branching, and spurious predictions. The field of nonlinear dynamics has introduced the phase portrait representation as a powerful tool for the global analysis of nonlinear differential equations. A state of the system is represented by a point in phase space; its behavior over time is represented by a trajectory. When the phase portrait is two-dimensional, the solutions to a differential equation can be characterized by the system's fixed points, bundles of adjacent trajectories (called flows), and certain bounding trajectories. Numeric methods for constructing phase portraits require numerically specific information about the system. We demonstrate a method and an implemented program, QPORTRAIT, that constructs two-dimensional phase portraits from QDE's. Starting with the total envisionment (a finite transition-graph representation of the possible behaviors of a system), QPORTRAIT progressively identifies, classifies, and combines features of the phase portrait, abstracting away uninteresting distinctions, and filtering out inconsistent combinations of features. Because each step in the analysis is validity-preserving, the prediction is guaranteed to cover all real phase portraits consistent with QDE. In its current form QPORTRAIT phase applies to a restricted but nontrivial set of QDE models. It requires that all fixed-points be non degenerate, and be at landmark values for the phase variables. QPORTRAIT has produced tractable results when applied to qualitative generalizations of several well-known nonlinear systems. Guaranteed coverage of the behavior of a qualitatively described set of QDE's complements the precision of numeric methods based approaches.

A qualitative method to construct phase portraits

Wood Wai Lee and Benjamin J. Kuipers
AAAI-93
AAAI/MIT Press, Cambridge, MA, 1993.

Abstract

We have developed and implemented a method based on qualitative simulation to construct phase portraits for a significant class of systems of two coupled first order autonomous differential equations, even in the presence of incomplete, qualitative knowledge. Differential equation models are important for reasoning about physical systems. The field of nonlinear dynamics has introduced the phase portrait representation as a powerful tool for the global analysis of nonlinear differential equations. QPORTRAIT uses qualitative simulation to generate the set of all possible qualitative behaviors of a system. Constraints on two-dimensional phase portraits from nonlinear dynamics make it possible to identify and classify the asymptotic limits of trajectories and constrain their possible combinations. By exhaustively forming all combinations of features, and filtering out inconsistent combinations, QPORTRAIT is guaranteed to generate all possible qualitative phase portraits. We have applied QPORTRAIT to obtain tractable results for a number of nontrivial dynamical systems. Guaranteed coverage of all possible behaviors of incompletely known systems complements the more detailed but approximation-based results of recently-developed methods for intelligently-guided numerical simulation [Nishida et al; Sacks; Yip; Zhao]. Together, these methods contribute to automated understanding of dynamical systems.

Behavior Abstraction for Tractable Simulation

Daniel J. Clancy and Benjamin Kuipers

Seventh International Workshop on Qualitative Reasoning (QR-93)

1993

Abstract

Most qualitative simulation techniques perform simulation at a single level of detail highlighting a fixed set of distinctions. This can lead to intractable branching within the behavioral description. The complexity of the simulation can be reduced by eliminating uninteresting distinctions. Behavior abstraction provides a hierarchy of behavioral descriptions allowing the modeler to select the appropriate level of description highlighting the relevant distinctions. Two abstraction techniques are presented. Behavior aggregation eliminates occurrence branching by providing a hybrid between a behavior tree representation and a history based description. Chatter box abstraction uses attainable envisionment to eliminate intractable branching due to chatter within a behavior tree simulation.

Model decomposition and simulation.

Daniel J. Clancy and Benjamin Kuipers.

Eighth International Workshop on Qualitative Reasoning (QR-94),

1994.

Abstract

Qualitative reasoning uses incomplete knowledge to compute a description of the possible behaviors for dynamic systems. For complex systems containing a large number of variables and

constraints, the simulation frequently is intractable or results in a large, incomprehensible behavioral description. Abstraction and aggregation techniques are required during the simulation to eliminate irrelevant details and highlight the important characteristics of the behavior. The total temporal ordering of unrelated events provided by a traditional state-based qualitative representation is one such irrelevant distinction. Model decomposition and simulation addresses this problem.

Model decomposition uses a causal analysis of the model to partition the variables into tightly connected components. The components are simulated separately in the order dictated by the causal analysis beginning with causally upstream components. Information from the simulation of causally upstream components is used to constrain the behavior of downstream components. If a feedback loop exists between components or a set of components are acausally related, then a concurrent simulation is performed for these components. A truth maintenance system is used to record and retract assumptions made during this concurrent simulation.

Model decomposition provides a general architecture which separates the method of simulation from the model decomposition algorithm. This architecture can be used to introduce alternative abstraction techniques to eliminate other irrelevant distinctions.

Guiding and refining simulation using temporal logic.

Giorgio Brajnik and Daniel J. Clancy

Proc. of the Third International Workshop on
Temporal Representation and Reasoning (TIME'96)
IEEE Computer Society Press, 1996.

Abstract

We illustrate TeQSIM, a qualitative simulator for continuous dynamical systems. It combines the expressive power of qualitative differential equations with temporal logic by interleaving simulation with model checking to constrain and refine the resulting predicted behaviors. Temporal logic expressions are used to specify constraints that restrict the simulation to a region of the state space and to specify trajectories for input variables. A propositional linear-time temporal logic is adopted, which is extended to a three valued logic that allows a formula to be conditionally entailed when quantitative information specified in the formula can be applied to a behavior to refine it. We present a formalization of the logic with theoretical results concerning the adopted model checking algorithm (correctness and completeness). We show also an example of the simulation of a non-autonomous dynamical system and illustrate possible application tasks, ranging from simulation to monitoring and control of continuous dynamical systems, where TeQSIM can be applied.

Temporal constraints on trajectories in qualitative simulation.

Giorgio Brajnik and Daniel J. Clancy.

Tenth International Workshop for Qualitative Reasoning (QR-96)

Fallen Leaf Lake, CA; May 1996.
AAAI Technical Report WS-96-01, pp.22-31.

Abstract

We present a new method for specifying temporal constraints on trajectories of dynamical systems and enforcing them during qualitative simulation. Such constraints are otherwise inexpressible using standard qualitative reasoning techniques. Trajectory constraints can be used to restrict the simulation to a region of the state space and to inject discontinuities. This capability can be used to focus the simulation for larger, more complex simulations, simulate non-autonomous and piecewise-continuous systems, reason about boundary condition problems and incorporate observations into the simulation. The method has been implemented in TeQSIM, a qualitative simulator. It combines the expressive power of qualitative differential equations with temporal logic by interleaving temporal logic model checking with the simulation to constrain and refine the resulting predicted behaviors and to inject discontinuous changes into the simulation.

The paper discusses the applicability of temporal constraints in tasks ranging from simulation to monitoring and control of continuous dynamical systems. We present a real-world control problem in the domain of water supply. Finally, the basic algorithm and theoretical results (soundness and completeness) are described.

2.5 Controller Verification Using Temporal Logic

The Composition and Validation of Heterogeneous Control Laws

B. J. Kuipers and K. Åström.

Automatica **30**(2): 233–249, 1994.

Abstract

We present a method for creating and validating a nonlinear controller by the composition of heterogeneous local control laws appropriate to different operating regions. Like fuzzy logic control, these methods apply even in the presence of incomplete knowledge of the structure of the system, the boundaries of the operating regions, or even the control action to take. Unlike fuzzy logic control, these methods can be analyzed by a combination of classical and qualitative methods. Each operating region of the system has a classical control law, which provides high-resolution control and can be analyzed by classical methods. Operating regions are defined by fuzzy set membership functions. The global control law is the weighted average of the local control laws, where the weights are provided by the operating region membership functions. A heterogeneous control law can be analyzed, even in the presence of incomplete knowledge, by representing it as a qualitative differential equation and using qualitative simulation to predict the set of possible behaviors of the system. By expressing the desired guarantee as a statement in a modal temporal logic, the validity of the guarantee can be automatically checked against the set of possible behaviors. We demonstrate heterogeneous controllers and our qualitative methods for proving their properties, first for a simple level controller for a water tank, and second for a highly nonlinear chemical reactor.

Qualitative simulation and temporal logic: proving properties of continuous systems

Benjamin Shults and Benjamin Kuipers.
University of Texas Artificial Intelligence Laboratory TR AI96-244,
January 1996

Abstract

We demonstrate an automated method for proving statements in temporal logic about continuous systems, even in the face of incomplete knowledge. The method combines an implemented, on-the-fly, model-checking algorithm for statements in the temporal logic CTL* [Bhat, et al, 1995; Clarke, et al, 1986; Emerson, 1990] with the output of the qualitative simulation algorithm QSIM [Kuipers, 1986, 1994]. Based on the QSIM Guaranteed Coverage Theorem, we prove that for certain CTL* statements, Φ, if Φ is true for the qualitative behavior tree produced by QSIM, then a corresponding theorem holds for the solution of any ordinary differential equation consistent with the qualitative differential equation that generated the QSIM behavior tree. We then show that for other CTL* formulas, if the QSIM output satisfies a certain completeness restriction, then conclusions can again be drawn about real-valued functions satisfying the given incomplete description. We also show how the methods can be applied to proving properties of continuous systems in which numeric information is available.