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ON THE POWER OF QUALITATIVE SIMULATION FOR ESTIMATING DIFFUSION TRANSIT TIMES

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ABSTRACT

Models describing the process of qualitative reasoning have significantly enhanced our insight into the general nature of the challenges involved in modeling people's imaginations when they think about complex processes. The composite picture created by combining models suggested by individual researchers may appear blurred This is because, in some cases, the range of applicability of each approach is not sharply defined, and the theoretical claims supporting the work are not sufficiently stated. This state of the art clearly suggests that considerable amount of research is still required in order to reinforce the theoretical foundations for the modeling qualitative reasoning. In this paper I first describe some of the approaches used for qualitative simulation. Second, I discuss present the example of diffusion process in complicated media and the challenges involved in automating the qualitative estimations of diffusion transit times.

1. INTRODUCTION

The ability to describe behaviors of dynamical systems is of great importance for explaining and predicting changes. In some cases, if the relationships which compose the system are simple enough, it may be possible to use analytic mathematical methods to arrive at the solution to the equations which describe these relationships. However, in the simulation of real-world systems, it is often the case that analytic solutions are out of the question and numerical simulation methods are used to generate behaviors of systems given a well defined set of initial and boundary values for the equations. Hence, numerical simulation methods are of great significance for gaining knowledge about the possible behaviors of a given model of a system for the chosen set of initial and boundary values. However, in many real life situations, it is often the case that not all the data needed to build a reasonably exact structural model of a system is available. Furthermore, in cases where systems are exceedingly complex, numerical simulations are highly cost ineffective, especially if what is sought after is the types of behaviors that this system can exhibit since, in such cases, many simulation runs have to be performed for different parameter ranges. Hence, in some of these cases it may be helpful to equipped the simulator with the ability to reason (simulate) qualitatively the behavior of the system and to explore the possible range of behaviors. In other words, the simulation process should include the utilization of commonsense knowledge about the process or the system being simulated.

The development of intelligent systems that perform complicated tasks such as qualitative reasoning, necessitates representing world knowledge in symbolic form. The essence of representing the knowledge is twofold: The content of the domain knowledge which is necessary to perform the task must be captured, and at the same time, this knowledge must be organized in a form which facilitates the task execution. Over the last decade, considerable research efforts in the field of Artificial Intelligence (AI) has been directed towards the automation of qualitative reasoning, with special emphasis on commonsense reasoning about physical systems. Qualitative reasoning programs have been developed to reason about electronic circuits (e.g. Davis 1984, Genesereth 1984), and everyday life physical processes (e.g. De Kleer and Brown 1984, Forbus 1984, Kuipers 1984). In addition, work has been done in a variety of other domains, such as medical diagnosis (e.g. Patil et al 1981), and the economy (Riesbeck 1984). For a survey of recent work see Chandrasekaran and Milne 1985 and Rajagopalan 1985.

The research reported here centers on the qualitative simulation of aspects of the process of diffusion in structured media. In particular, I am interested in the automation of reasoning about the effect that the geometry of the diffusion space and its composition have on the diffusion transit time. To demonstrate the issues involved, consider the following problem:

Molecules released from the surface on the left diffuse to, and are trapped by the surface on the right. The molecules are slightly soluble in water, and highly soluble in oil. In case (a) they diffuse through the layer of oil before reaching the layer of water. In case (b) the thickness of each layer is unchanged but the order is reversed so the molecules diffuse first through the water and then the oil. Compare the transit times.

The same in both	[ ]
Much longer in (a)	[ ]
Much longer in (b)	[ ]

(a) (b)

Numerical simulation of the problem presented in the quiz question above is highly expensive. In addition, since all we are interested in, in this case, is a qualitative comparison between the average diffusion time in the two cases, an exact numerical simulation of the diffusion equation, can not give us the answer directly, and in addition, this solution method generate too much information that is beyond the scope of the problem. In some sense, all one needs to solve this problem is intuition about diffusional processes and some heuristics (rules of thumb) to guide the qualitative reasoning. In Hardt 1980b, and Hardt 1984, exact solution to the transit time and helpful heuristics are presented. The problem I am addressing here is how to represent these commonsense knowledge in a way that a machine can use in order to solve this and similar problems.

In the following the AI approaches to the automation of qualitative reasoning are briefly described together with an outline of a solution to the above quiz problem.

2. APPROACHES TO QUALITATIVE SIMULATION

Research in AI is aimed at extending the capabilities of machines to perform computation of the kind people perform when they deal with task domains in the real world. Furthermore, AI research attempts to explore the nature of human thinking, and to build cognitively valid computer models. Naturally, these two aims are not mutually exclusive. AI research directed at understanding and modeling qualitative reasoning, concentrates mainly on: (a) deriving the qualitative concepts used in formal models if they exist, and (b) identifying the core knowledge underlying intuition in the domain (see Hayes 1985).

There is a great similarity between building a simulation model and building a knowledge base. The descriptions of natural phenomena or artificial systems can be organized by the logical discipline of Mathematics. When mathematics is applied to problems in the natural world, the resulting formulation is rich with the mathematician intuition. The thought processes that resulted in the formulation are, in an important sense, incorporated in it. There application of Mathematics involves a few steps (e.g. Lin and Segel 1974). First, the *formulation* of the scientific problem in mathematical terms. Second, the *solution* of the mathematical problems. And third, the *interpretation* of the solution and its empirical verification in scientific terms. Each of these steps involves a translation of reality into a different vocabulary.

The above description of the formulation of mathematical models of observed phenomena is a simplification to a rather complex cognitive process in which the scientist uses his native commonsense combined with the thinking tools provided by his training in the discipline of mathematics, to produce a formal model. If we now compare this process of model formation to the one employed by a person who has no training in mathematics, but who has to build some models of reality in order to function in everyday life situations, we may discover that the latter are amazingly effective and can produce relevant results for complex situations, in real-time. It is beyond the scope of the current paper to go in depth into a comparative discussion on the nature of the formalism of thought and the formalism of mathematics. For our purposes here, it is sufficient to conjecture that the two formalisms are different in scope and purpose.

Given the above distinction between mathematical and cognitive models of a process , we can now perceive some of the different ways one can go about building a qualitative simulation model. There are two basics approachs on can take. One approach is to simplify the exact mathematical equations describing the system and replace them with qualitative equations. This approach is central to the work of De Kleer and Brown 1984, and Kuipers 1984. The second approach to building qualitative reasoning systems is to construct the cognitive (commonsense) models that a person uses to reason about the processes under consideration. This approach is used to different extents by various researchers in AI and Cognitive Science. In particular it is central to the work of Hayes 1985, Forbus 1984, Bylander and Chandrasekaran 1985, Gentner and Gentner 1983 and Hardt 1984.

In general, qualitative simulation captures less detail and therefore may produce partial behavioral descriptions. Also, the quantitative precision of these descriptions is reduced while crucial distinctions are retained. However, it is important to notice that in fields of scientific enquiry where exact models are desirable, many of the basic concepts are qualitative. For example, in Classical Physics, concepts like state, law, cause, equilibrium, oscillation, momentum, feedback, etc. are qualitative in nature, and they have been embedded in a complex framework established by the Mathematics of real numbers and differential equations.

3. DIFFUSIONAL PROCESSES AND COMMONSENSE

Building a qualitative reasoning system for reasoning about diffusional process is a complicated task. The complexity of the dynamics of diffusion is hard to describe intuitively and hence, powerful commonsense models are possessed by only a few experts. In addition, most of the reasoning about diffusion involves taking into account some averaging of complicated behaviors of many objects (particles) over long periods of time.

Mathematically, there are different levels of description from which the physical process of diffusion can be formally described. Three of these levels are: 1. The level of individual particles. This level is presentable by the mathematical theory of stochastic processes. 2. The level of small collections of particles. In this context the notion of concentration is introduced and its dynamic behavior expressed in terms of partial differential equation. 3. The thermodynamic level where the notion of entropy is introduced. Each level of description has its own vocabulary and set of relations.

Although these formal levels of description are based on reasonably sound mathematical theories, they are not suited, in many cases, to serve as foundations for commonsense knowledge about diffusion. It is important to keep in mind that as far as common sense understanding is concerned, the rules of thumb use a mixed level vocabulary (see for example Hardt 1980b and later this paper). A similar point is made by Feynman et al, 1963, when it is stressed that framing a physical description of a system of particles and their interaction, must start with a consideration of the hierarchical structure of possible descriptions. Only in the context of such a hierarchy, he emphasizes, do basic concepts, like frictional force, conservative force, kinetic energy and potential energy, assume precision. This can be abstracted to any system composed of modules.

In the work reported here, the reasoning system is confronted with the task of reasoning about and estimating the pace of diffusional flow inside complicated channels. This process appears continuous in time and space yet its pace is crucially dependent on the shape size and texture of the channel. The ability to reason about the pace of this flow process originates directly from detailed knowledge about the process.

4. QUALITATIVE ESTIMATION OF DIFFUSION TIMES

The duration of complex events can not be estimated in a straightforward fashion. Events may partially overlap in time, consecutive events may be delayed, side-effects may interfere to alter the pace of future events, and so on. The discussion here is limited in focus to the cognitive process of estimating the duration of events that take place in the physical world, and therefore, this work can be characterized as naive physics. Limiting the repertoire of events to physical events, namely to events that do not include human intention, simplifies the task of time estimation considerably, as one need not worry about the effectiveness of individual human actors to formulate a goal, to plan for a known goal, to perform a planned action or to react to a given action. However, even with this simplification, the computational task is far from simple.

It goes without saying that in order to estimate event durations, a system must have detailed knowledge about the dynamical behavior of the processes which cause the event. However, there are important questions that have to be addressed before such knowledge can be effectively made available to any reasoning system. For example, the question of event interpretation and analysis; given an event description, how to break this event into sub-events corresponding to some (primitive) events of known duration. This question is closely related to the question of how to determine what are the appropriate reasoning steps during qualitative reasoning using deep causal models. In order to apply this particular method of problem solving, the reasoning system has to possess the knowledge on how to decompose the process into more primitive processes of known characteristics that take place in sub-regions of the system. Part of the systems knowledge base is listed informally below that should be used to solve the quiz and similar problems (see Hardt 1984 for a list of problems and see Hardt 1979, 1980a, 1980b for the source of the rules).

Rules for identifying sub-regions:

Rule 1: Different media (compositions) define regions.
Rule 2: Dimensionality of the movement defines regions.
Rule 3: The target defines a region (scaled appropriately).
Rule 4: The source defines a region (scaled appropriately).
Rule 5: The rest of the system defines a region (scaled appropriately).

Principles of the process:
Basic Property 1: Particles move randomly (equal chances to go left and right in each dimension).
Basic Property 2: Each degree of freedom is independent.
Basic Observation 1: Since diffusing particles look for the target randomly, if they spend more time in the region near it, they are more likely to find it.
Basic Effect 1 (Dimensionality effect): The higher the dimensionality of the diffusion space, the harder it is to find a point in that space.
Basic Effect 2 (Media effect): The greater the affinity of the particle to a particular media the more time it will spent there.

In many cases, it is possible to decompose the system in more than one way. Therefore, the sub-region recognition rules are implemented as parallel processes, each pursuing its own interpretation and estimation of the process.

5. CONCLUDING REMARKS

There are many intriguing high level questions that have to be addressed before a reasonably sound theoretical framework can be developed for modeling qualitative reasoning. Among this questions are:
1. Types of mechanisms for qualitative reasoning and their cognitive validity.
2. Reasoning styles and their impact on reasoning effectiveness.
3. The power of qualitative reasoning.
4. Ways to incorporate qualitative reasoning in real-time problem solving.

The research in-progress reported here is aimed at gaining insight into these issues by dealing with a complex reasoning problem for which an exact mathematical formulation exists and in which problem solving can be aided by expansive numerical simulations and by fast and effective commonsense reasoning.

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