Qualitative Reasoning with Microscopic Theories

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Abstract

A model of the elementary particles of a domain and their rudimentary interactions is essential for sophisticated reasoning about the macroscopic behavior of physical system. A microscopic theory can make explicit the deeper mechanisms underlying causal models, collapse a great variety of macroscopic phenomena into a few rudimentary interactions, elaborate upon or validate macroscopic explanations, and so forth. This paper describes a qualitative representation for microscopic theories and, a method for reasoning with microscopic particles to obtain the macroscopic behavior. The representation and reasoning are illustrated using implemented examples from the fluids domain.

Introduction

A central goal of Artificial Intelligence (AI) is to build systems that are capable of expert performance. Early expert systems were based on domain models that encoded empirically observed associations as rules (for example, MYCIN [Shortliffe 76]). However, these shallow models failed to capture the causal relations underlying the rules; consequently, they were severely limited in their explanatory capabilities. Later AI methods, model-based reasoning [Davis 88] and, more specifically, qualitative reasoning [Forbus 84, de Kleer & Brown 84, Kuipers 86], use a deeper model of the domain that captures many of the underlying causal relations in the form of incompletely specified constraints. While qualitative reasoning systems demonstrate improved performance, the explanations they provide are often inadequate since they lack a deeper theory underlying their causal models.

A profound understanding of the domain in terms of a theory of the elementary particles comprising the domain and their interactions is a prerequisite to superior explanatory performance since these rudimentary interactions define the observed macroscopic behavior. A theory of elementary particles can make explicit the deeper mechanisms underlying the causal relations; collapse a great variety of macroscopic phenomena into a few rudimentary interactions; determine the effect of perturbations on factors affecting the causal relations; elaborate upon or validate macroscopic explanations; explain phenomena such as Brownian motion that are direct manifestations of the microscopic world; and so forth.

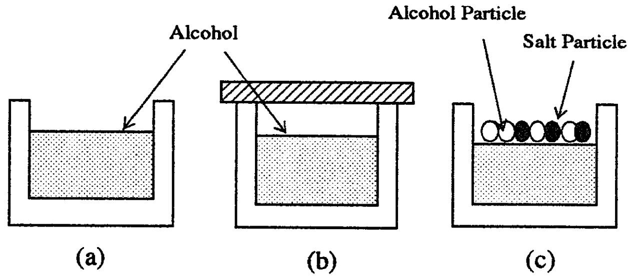

Figure 1: Situations involving microscopic reasoning.

This paper describes a qualitative representation for microscopic theories and a method for reasoning with them. The representation carves the macroscopic world into a small number of hypothetical particles representative of collections of actual particles. Reasoning considers the effect of rudimentary interactions on these hypothetical particles, and extends the results to the collections associated with them in accordance with the laws pertaining to the distribution of the particles. Finally, the computed microscopic behavior is mapped back to the macroscopic world to provide explanations for the observed macroscopic behavior. Implemented examples from the fluids domain are used to illustrate the representation of, and the reasoning with, microscopic theories.

Motivating Examples

This section describes several situations that require reasoning with microscopic theories. These examples illustrate the importance and the utility of microscopic theories.

Profound Explanations. Consider the simple situation shown in Figure 1a in which some alcohol is placed in an open container. Why does the temperature of the alcohol drop? A simple explanation is:

> The contained alcohol is exposed to the external atmosphere; consequently, it evaporates. Evaporation leads

to the drop in the temperature of the alcohol.

A more profound explanation is:

> The kinetic theory of fluids [Lee 70] postulates that the molecules of the alcohol contained in the open bowl are continually in random motion, and are held together by intermolecular forces of attraction. According to the random distribution of energies, some of the molecules may have high kinetic energy. Some of these molecules may possess sufficient energy to conquer the forces of attraction. If some of them are on the surface and have outward velocity, they escape from the liquid and are lost to the external atmosphere. The constant loss of such high energy molecules leads to a drop in the average kinetic energy of the molecules. Since the macroscopic property, temperature, is directly proportional to the average kinetic energy of liquid particles, the temperature of the alcohol will drop.

The first explanation is based on empirically observed relations such as "evaporation occurs when a liquid is exposed to the external atmosphere, and it results in a drop in the temperature of the evaporating liquid." The second explanation is a deeper explanation that involves more fundamental concepts, and displays a profound understanding of the nature of matter, its constituents, and the interactions among them.

Dynamic Equilibria. Consider what happens when the bowl of alcohol is closed completely (Figure 1b). Eventually, the level and the temperature of the enclosed alcohol become constant; outwardly, it appears as though all activity has ceased. However, the picture at the microscopic level is one of continuous raging activity; but, in this case, the escape of high-energy molecules is matched by the capture of molecules from the atmosphere. The understanding of such dynamic equilibria at the microscopic level is instrumental in explaining many otherwise mysterious phenomena like diffusion and osmosis.

Mechanisms of Processes. What is the effect of dissolving a salt in the alcohol (Figure 1c)? How does the rate of evaporation vary with the concentration of the solution? A microscopic theory makes explicit the mechanism underlying evaporation. A microscopic model for evaporation will describe it as the escape of liquid molecules from the surface, and will predict a drop in the rate of evaporation with dissolving since the solute[1] particles deprive the solvent particles of many escape sites by occupying a portion of the alcohol's surface. Therefore, as the concentration of the solution increases the rate of evaporation will drop.

The Architecture of MRE

Figure 2 shows the architecture of the implemented microscopic reasoning system, MRE[2]. The inputs to the

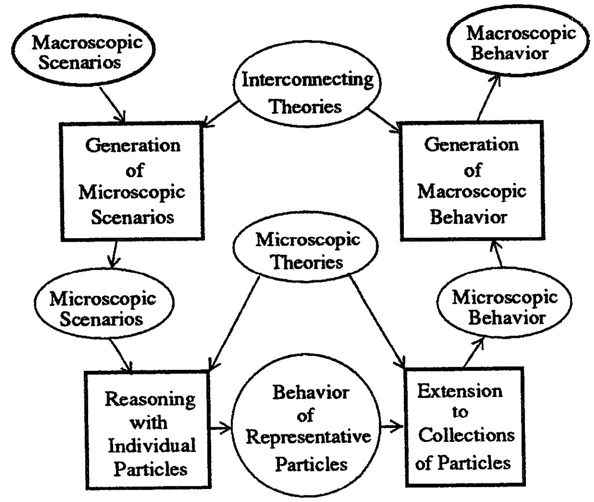

Figure 2: Architecture of the MRE system

system are the macroscopic description of a situation of interest from the domain (whose behavior is to be determined) and, macroscopic and microscopic theories of the domain that describe the objects in the domain, their interactions, and the relationship between the two theories. The outputs of the system are the macroscopic and microscopic behavior of the situation,[3] and explanations for the behavior. The system converts the macroscopic scenario into a microscopic representation involving representative particles, reasons about the interactions among these particles, extends the results to the collections of particles associated with them and, finally, computes the macroscopic changes due to these microscopic changes.

Representation of Microscopic Theories

The representation of microscopic theories includes the representation of the microscopic particles, their interactions, and the relationship between the macroscopic and microscopic theories. Despite the seemingly unnerving complexity of the billions and billions of particles at the microscopic level, reasoning at this level is not impossible because there are only a few qualitatively different interactions, and each interaction involves a few particles belonging to qualitatively distinct groups. Therefore, an important function of a representation of microscopic theories is to identify and distinguish between these particles.

Microscopic Particles. We define three types of hypothetical particles that serve as representatives for groups of microscopic particles: (a) *Average Particle.* An average particle represents the entire collection of

[1] A solution consists of two components: a liquid *solvent* and a solid *solute*.

[2] The MRE system is a rule-based qualitative simulator with an underlying ATMS [de Kleer 86].

[3] The current implementation of the system obtains only the behavior for the initial state. It does not compute the *envisionment* [de Kleer & Brown 84, Forbus 84] or how the behavior evolves over time. We are in the process of extending the implementation to obtain the envisionment too.

particles that make up a macroscopic object. Often, this hypothetical particle suffices for many situations, for instance, a flow of a liquid through a pipe under external pressure. (b) *Qualified Particle.* An average particle is further qualified to take into account its type. A macroscopic object may be composed of various kinds of particles. For example, a solution consists of solute particles and solvent particles. Qualified particles are necessary to reason about phenomena such as osmosis that preferentially involve one type of particle. (c) *Quantified Particle.* An average particle of a particular type need not describe a group of uniform particles. The particles within each group may have widely differing values for properties such as kinetic energy, velocity, and momentum. Quantified particles capture the qualitative differences in the values of these properties. The particles are divided along the dimensions of the quantity spaces [Forbus 84] for each continuous quantity and the property spaces for other properties (such as *outward-velocity* and *on-surface*) and a quantified particle is associated with each division. Quantified particles are useful in reasoning about phenomena such as evaporation that involve particles with kinetic energy greater than the forces of intermolecular attraction (barrier energy).

Consider the situation shown in Figure 1c. The macroscopic object, the contained solution consisting of some salt dissolved in the alcohol, will have one representative, hypothetical particle—*contained-solution-average-particle.* This average particle is divided into two kinds of qualified particles, solvent and solute particles. The solvent particle is further divided into several kinds of quantified particles: for example, a *high-kinetic-energy-particle* (with kinetic energy greater than the barrier energy) and a *low-kinetic-energy-particle* (with kinetic energy less than the barrier energy).

Rudimentary Interactions. The representation of rudimentary interactions includes a description of the particles that may participate, the conditions that the particles must satisfy, and the effects of the interaction. Our representation is similar to the *process* representation in QP theory; however, in our case, the effects may include discrete changes, such as a phase transition from a liquid particle to a gas particle with escape, in addition to continuous changes like a decrease in kinetic energy of a particle. Table 1 shows the representation for the rudimentary interaction **escape** of a liquid particle.

We define two additional quantities for reasoning about many instances of the same interaction on different particles drawn from the groups associated with the representative particles: (1) *Population.* The population of a particle (average, quantified, or qualified) represents the population of the group of particles associated with the representative particle. The population of the average particle of a macroscopic object represents the entire collection of particles that constitute the object. (2) *Frequency.* Frequency corresponds to the number of instances of an interaction that are active. It is analogous to the macroscopic quantity, the *rate* of a process, in Forbus' QP theory. As is normally the case in qualitative reasoning, we are not concerned with the numerical values of these quantities, but only with their relative magnitudes.

Rudimentary Interaction: Escape (?liq-particle)	
Individuals :	
?liq-particle	; a representative particle of the contained-liquid
QuantityConditions :	
kinetic-energy(?liq-particle) > barrier-energy(?liq-particle)	
Preconditions :	
outward-velocity(?liq-particle)	
on-surface(?liq-particle)	
Results :	
phase-transition	(?liq-particle, liquid, gas)
location-transition	(?liq-particle, on-surface, in-gas)

Table 1: Rudimentary interaction **Escape**.

The frequency of an interaction and the population of the pools from which the participating particles are drawn are related. Consider the **escape** interaction previously described. The frequency of **escape** is qualitatively proportional to three quantities: the population of the high-kinetic-energy liquid particles, the population of the liquid particles on the surface, and the population of the liquid particles with outward velocity. Dissolving a substance in the liquid will decrease the population of the liquid particles on the surface leading to a decrease in the frequency of **escape** (manifested as a decrease in the rate of evaporation in the macroscopic world). **Escape** results in a decrease in the population of the high-kinetic-energy particles, and this too will lead to a decrease in the frequency of **escape**.

The Interconnecting Theory. The interconnecting theory describes the relationship between the macroscopic and microscopic worlds, and is needed to obtain the microscopic description of the scenario from the given macroscopic description, and to obtain the macroscopic behavior from the computed microscopic behavior. For the former task, the interconnecting theory must specify the composition of the macroscopic objects in terms of microscopic particles, and the quantity relations among the populations of the different types of particles constituting the object. For the latter task, the interconnecting theory must specify the relationship between the macroscopic and the microscopic quantities.

Table 2 shows the parts of the interconnecting theory required to generate the microscopic descriptions for the contained alcohol in the situation shown in Figure 1a. The theory specifies that a liquid consists of liquid particles, some of which are on the surface and some of which are in the interior. At any time, the number of

```
Macroscopic-Object: Contained-Liquid(?contained-alcohol)
Average-Particle :average-particle
Quantified-Particles :
  outward-particle               ; a particle with outward velocity
  inward-particle                ; a particle with inward velocity
  on-surface-particle            ; a particle located on surface
  interior-particle              ; a particle located inside the liquid
  high-kinetic-energy-particle   ; a high kinetic energy particle
  low-kinetic-energy-particle    ; a low kinetic energy particle
  ....
Relations :
  population(on-surface-particle) = constant
  population(average-particle) Q= population(outward-particle)
                               + population(inward-particle)
  population(average-particle) Q= population(on-surface-particle)
                               + population(interior-particle)
  kinetic-energy(average-particle) Q+
                               population(high-kinetic-energy-particle)
  kinetic-energy(average-particle) Q-
                               population(low-kinetic-energy-particle)
  temperature(?contained-alcohol) Q+ kinetic-energy(average-particle)
  amount(?contained-alcohol) Q+ population(average-particle)
  ....
```

Table 2: The interconnecting theory corresponding to the macroscopic entity *contained-alcohol.*

particles on the surface is constant[4]—so if a particle escapes, a particle from the interior must occupy its space. In addition, it specifies that at a given time, half the particles will have outward velocity and the remaining half will have inward velocity. The description also specifies the relationships between the amount of the contained liquid and the population of the average particle, and between the temperature of the contained liquid and the kinetic energy of the average particle.

Microscopic Reasoning

The qualitative simulation of a given macroscopic scenario proceeds in four steps:

1. *Moving down to microscopic world.* The given macroscopic scenario is first converted into a microscopic representation. For each macroscopic object, the corresponding hypothetical particles: average, qualified, and quantified are created, and the relations due to these particles are asserted. Also, in this step, the quantity relations among the populations of the different types of particles are also asserted.
2. *Reasoning with the representative particles.* The representative particles are examined to check if a group of representative particles satisfies the requirements of any of the rudimentary interactions. If a given group does satisfy the requirements, the rudimentary interaction is asserted to be active, and all the effects of the interaction are asserted.
3. *Extending the reasoning to collections of particles.* Using the notions of population and frequency, the results of the previous stage are extended to the collections of particles associated with each of the representative particles. The frequency of each of the active rudimentary interactions is determined based on the populations that affect it, and the changes to the frequency are determined by computing the changes to the populations due to the interactions. At the end of this step, the microscopic behavior of the scenario is fully determined.
4. *Moving back to macroscopic world.* Finally, the microscopic behavior is converted into observable macroscopic behavior using the relations postulated by the interconnecting theory. At the end of this step, the macroscopic behavior of the given scenario is determined, and profound, microscopic-level explanations are available for each of the predicted changes.

Consider the situation shown in Figure 1a involving the evaporation of the contained alcohol. The MRE system is given a macroscopic description of the situation: in this case, there are two macroscopic entities—the contained alcohol and the contained vapor.[5] The first step generates the representative particles corresponding to each of the macroscopic entities. The second step examines collections of particles to check if they can participate in a rudimentary interaction. In this case, an alcohol particle that is on the surface, has outward velocity, and possesses kinetic energy greater than the barrier energy participates in the **escape** interaction. The interaction results in a phase transition of the particle from the liquid to the gaseous state. The third step computes the effects of many such interactions. The frequency of **escape** depends on the populations of three types of particles: the alcohol particles on the surface, the alcohol particles with outward velocity, and the alcohol particles with kinetic energy greater than the barrier energy. Since **escape** results in a decrease in the population of the last group, the frequency of **escape** gradually drops. The last step maps the changes at the microscopic level onto macroscopic quantities. A decrease in the population of the average particle for alcohol corresponds to a decrease in the amount of the alcohol. Likewise, a decrease in the kinetic energy of the average particle results in a drop in the alcohol temperature. Table 3 shows the (truncated) explanation for the decrease in the temperature of the alcohol.

Additional Examples

In this section, we briefly describe two additional implemented examples involving the situations shown in Figures 1b and 1c that were described in Section 2.

[4] This model assumes that the amount of liquid is at all times sufficient to form a complete surface spanning the width of the container. A small drop of liquid in the container will not be consistent with this model as its surface will change with evaporation.

[5] As in [Hayes 85, Forbus 84], we use the Contained-Liquid ontology to specify macroscopic objects.

```
(⇓ (temperature alcohol))
    (Q+ (temperature alcohol) (KE aver-alcohol-p))
        (Active contained-alcohol)
    (⇓ (KE aver-alcohol-p)))
        (Q+ (KE aver-alcohol-p) (pop high-KE-alcohol-p))
            (Active aver-alcohol-p)
        (⇓ (pop high-KE-alcohol-p))
            (Q+ (pop high-KE-alcohol-p) (pop escape-p))
                (Active high-KE-alcohol-p)
            (⇓ (pop escape-p))
                (> (A (freq (escape escape-p))) 0)
                    (phase-transition escape-p liquid gas)
                        (Active (escape escape-p))
                (I- (pop escape-p) (A (freq (escape escape-p))))
                    (Active (escape escape-p))

Description of particles involved in explanation.
aver-alcohol-p = (aver-p (CL alcohol))
high-KE-alcohol-p = (quantified-p (aver-p (CL alcohol))
                        (> (A (KE (aver-p (CL alcohol))))
                           (A (BE (aver-p (CL alcohol))))))
escape-p = (quantified-p (aver-p (CL alcohol))
                        (on-surface (aver-p (CL alcohol)))
                        (outward-velocity (aver-p (CL alcohol)))
                        (> (A (KE (aver-p (CL alcohol))))
                           (A (BE (aver-p (CL alcohol))))))

*note :  ⇓ (decreasing)
         ⇑ (increasing)
         p (particle)
         KE (kinetic-energy)
         BE (barrier-energy)
         CL (contained-liquid)
         pop (population)
         freq (frequency)
```

Table 3: The explanations for a drop in the alcohol temperature. The explanations for why the particles are active is not shown.

```
(⇑(freq (capture capture-p)))
    (Q+ (freq (capture capture-p)) (pop aver-gas-p))
        (active (capture capture-p))
    (⇑(pop aver-gas-p))
        (Q+ (pop aver-gas-p) (pop capture-p))
            (active aver-gas-p)
        (⇓ (pop capture-p))
            (> (A (freq (capture capture-p))) 0)
                (phase-transition capture-p gas liquid)
                    (active (capture capture-p))
            (I- (pop capture-p) (A (freq (capture capture-p))))
                (active (capture capture-p))
        (Q- (pop aver-gas-p) (pop escape-p))
            (active aver-gas-p)
        (⇓ (pop escape-p))
            (> (A (freq (escape escape-p))) 0)
                (phase-transition escape-p liquid gas)
                    (active (escape escape-p))
            (I+ (pop aver-gas-p) (A (freq (escape escape-p))))
                (active (escape escape-p))
        (> (pop escape-p) (pop capture-p))


(⇓ (freq (escape escape-p)))
    (Q+ (freq (escape escape-p)) (pop on-surface-alcohol-p)))
        (active (escape escape-p))
    (⇓ (pop on-surface-alcohol-p))
        (Q+ (pop on-surface-alcohol-p) (pop escape-p))
            (active on-surface-alcohol-p)
        (⇓ (pop escape-p))
            (> (A (freq (escape escape-p))) 0)
                (phase-transition escape-p liquid gas)
                    (active (escape escape-p))
            (I- (pop escape-p) (A (freq (escape escape-p))))
                (active (escape escape-p))
```

Table 4: Explanations for some of the changes in the situations shown in Figures 1b and 1c.

The first explanation in Table 4 describes the tendency of the rates of evaporation and condensation to attain equilibrium in a closed container (please refer to the situation shown in Figure 1b). It is initially assumed that the rate of evaporation is greater than that of condensation. The explanation describes why the frequency of the **capture** of the gas particles gradually increases due to an increase in the population of gas particles (which in turn is due to evaporation dominating condensation). A similar explanation for why the frequency of the **escape** of the alcohol particles gradually drops is constructed by the system. As yet, the current implementation of MRE does not perform *limit analysis* [Forbus 84], therefore, it cannot describe the attainment of the dynamic equilibrium.

The second explanation in Table 4 describes why the rate of evaporation gradually drops in the situation of Figure 1c. In this case, alcohol particles satisfying the requirements of the **escape** interaction: namely, they must be on the surface, have outward velocity, and possess sufficient kinetic energy to overcome the barrier, are constantly lost. The frequency of **escape** depends on the populations of the collections of particles satisfying these requirements. The explanation shown in the table describes why the frequency of **escape** drops because the population of the alcohol particles on the surface drops (the additional explanation for the drop in frequency due to the depletion of high-kinetic-energy alcohol particles is not shown). Note that the population of the particles on the surface is maintained constant by a corresponding increase in the population of the salt particles on the surface.

Related Research

Research on qualitative reasoning has traditionally focused on reasoning with macroscopic theories [Forbus 84, de Kleer & Brown 84, Kuipers 86]. Hayes [Hayes 85] has developed two types of ontologies to describe the behavior of liquids: the *contained-liquid* ontology and the *piece-of-stuff* ontology. Collins and Forbus [Collins & Forbus 87] have further expanded the piece-of-stuff ontology to their *molecular collection* ontology. The contained-stuff and the piece-of-stuff ontologies reason with complementary perspectives of a phenomenon at the macroscopic level: the former reasons about the changes to a liquid defined by its containment in a vessel, and the latter reasons about changes to a liquid during its movement through a system. The MRE system, on the other hand, reasons about a physical phenomenon with two theories at different levels of abstraction—the macroscopic and the microscopic levels. Unlike our quantified-particles representation, the piece-of-stuff and molecular collection ontologies assume a distribution of uniform pieces and, consequently, cannot explain phenomena like evaporation that involve reasoning about the differences in the pieces. Collins and Forbus compute the behavioral description of their molecular collections from the macroscopic behavior and from annotations to macroscopic processes, whereas the MRE system uses separate representations for the microscopic theories and macroscopic theories, and links the two theories using an interconnecting theory.

A number of researchers have used multiple theories or levels of abstraction in reasoning and learning. For example, Doyle [Doyle 86] describes a learning system that uses multiple theories at different levels of generality. Weld [Weld 86] describes a system that forms abstractions via aggregation. However, these researchers have not dealt with microscopic theories which have unique problems due to the large number of particles and the transitory nature of their individual behavior.

Discussion

Microscopic theories are of considerable importance in the understanding and explication of many physical phenomena. This paper has described an initial step towards the qualitative representation of, and the reasoning with, microscopic theories. The representation defines a small number of hypothetical representative particles for a macroscopic object. Reasoning commences by converting the given macroscopic representation into a microscopic one by identifying the representative particles for each macroscopic object, and by asserting the relationships among the particles that hold in the given situation. Next, the rudimentary interactions that are active are determined and their results are asserted. Reasoning then extends these results for the collections of particles associated with each of the representative particles to obtain the microscopic behavior. The final step involves converting the microscopic behavior into the macroscopic behavior using the interconnecting theory. The implemented system, MRE, was demonstrated on several examples from the fluids domain.

The present framework suffers from many limitations that restrict the types of microscopic theories that can be represented and reasoned with: for example, it lacks a sophisticated geometric reasoner, a good representation for motion (including random motion, vibration, etc.), and a good representation for forces (including intermolecular forces of attraction in liquids). Apart from addressing these limitations, we envisage several important directions for future research: (1) Envisionment: We are currently extending the current implementation to construct an envisionment at the microscopic level. This will enable us to reason about phenomena involving dynamic equilibria such as the one described in Section 2. (2) Integrated reasoning: We plan to draw on the strengths of macroscopic and microscopic reasoning to overcome their respective limitations. (3) Learning: We plan to extend our earlier research on learning macroscopic theories of physical phenomena [Rajamoney 90] by incorporating microscopic theories to validate and extend the learned macroscopic theories.

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