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THE INTERDEPENDENCIES OF THEORY FORMATION, REVISION, AND EXPERIMENTATION

by

Brian Falkenhainer
Shankar Rajamoney

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This paper depicts theory development as a synergistic cooperation of scientific methodologies, each focusing on different aspects of the problem. It discusses how they may be integrated to provide a more unified and comprehensive treatment of scientific theory discovery. ~~We describe~~ is described a general protocol for interaction between theory formation, theory revision, and experimentation. This protocol enables theory formation to make specific queries about the state of the world to fulfill its hypothesis generation goals. It also enables epxerimentation-based revision to post tasks for theory formation to supply relevant hypotheses. The utility and generality of this protocol is demonstrated by an implementation which integrates two previously autonomous systems. Its performance is described for discovering and revising models of evaporation and osmosis.

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THE INTERDEPENDENCIES OF THEORY FORMATION, REVISION, AND EXPERIMENTATION

by

Brian Falkenhainer
Shankar Rajamoney

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Department of Computer Science
University of Illinois at Urbana-Champaign
1304 W. Springfield Avenue
Urbana, Illinois 61801

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1. Introduction

Scientific discovery follows a cyclic pattern of theory development – the formation of a new theory, a number of fixes to account for anomalous behavior and, later, when the fixes result in a grossly inelegant theory, a paradigm shift that radically transforms the old theory (Kuhn, 1970). Theory development is a multi-faceted process involving the synergistic cooperation of a number of approaches. This paper attempts to provide a comprehensive model for each stage of theory development by integrating several techniques – empirical learning, analogical learning, and experimentation.

Our central task is to provide causal explanations of observed natural phenomena, using an imperfect or non-existent theory of the domain. This paper describes the integration of two techniques: *verification-based analogical learning*, which is used primarily for theory formation (including paradigm shifts), and *experimentation-based theory revision*, which is used primarily for theory testing and revision. (We review each only briefly here, for details see (Falkenhainer, 1987) and (Rajamoney, 1988)). Analogy-driven theory formation can develop novel theories in a focused manner, drawing from its knowledge of analogous precedents. However, in isolation it lacks the ability to examine the state of the world and experimentally confirm or refute hypotheses. Experimentation-based theory revision, on the other hand, is well suited to modifying theories and testing the different modifications to a theory. However, it has very little guidance during the task of proposing different modifications to a theory. Also, it must rely on fortuitous observations or prediction failures to initiate theory revision.

In this paper, we describe a set of general principles underlying theory formation, theory revision, and experimentation. We demonstrate how these techniques, each focusing on different aspects of the problem, may be integrated to provide a more unified and comprehensive treatment of scientific theory development. In particular, we show how experimentation is used to empirically guide and verify the analogy-driven theory formation stage and how analogy is used to initiate and focus the experimentation-based theory revision stage. Furthermore, we outline a general protocol for communication between theory formation and experimentation-based revision which solves many of their individual problems. Experimental queries using the protocol are motivated by empirical questions and requirements encountered during hypothesis generation and evaluation. Theoretical queries are motivated by the need for plausible hypotheses during experimentation-based theory revision.

The utility and generality of this protocol is demonstrated by an implementation integrating two previously autonomous systems: PHINEAS, which performs verification-based analogical learning, and ADEPT, which performs experimentation-based theory revision. When confronted with a novel observation of evaporation, this integrated architecture and its associated protocol enabled PHINEAS to empirically question the necessity of heat flow (e.g., from a stove) in its evaporation hypothesis derived from boiling. In turn, the protocol enabled ADEPT to be advised of vapor saturation as a candidate explanation for why evaporation stopped.

We conclude this section with a review of the two techniques. An integrated design and the general principles which emerge is then described in section 2 and made concrete with the use of an implemented example. An additional example is briefly provided in section 3.

1.1. Verification–Based Analogical Learning: An Overview

Verification–based analogical learning (VBAL) (Falkenhainer, 1987) is an approach to theory formation and revision which relies on analogical inference to hypothesize new theories, and *gedanken* experiments (i.e., simulation) to analyze their validity. VBAL is an iterative process consisting of four primary stages:

1. **Behavior match.** An anomalous observation triggers a search for previously understood experiences that exhibited analogous behavior. The result of this stage is a candidate analogue and an initial set of correspondences between the two domains.[1]
2. **Theory generation.** The central objective of the second stage is to produce a fully operational initial hypothesis about the current domain. This stage has two components. First, the model used to explain the recalled experience is analogically mapped into the current domain. This mapping is guided by the initial correspondences found in the behavioral comparison. Second, the model must be *operationalized* if it is not already. For example, it may reference entities and properties that are currently unknown. These entities and properties must either be inferred from the domain theory or their existence must be postulated.
3. **Theory completion.** The operational model may not necessarily conform to the present observation. Thus, theory revision may be required to examine predictions and produce a consistent initial model. Revision in VBAL is based on passive consistency – when empirical experiments are impossible, prefer minimal revisions with an analogical precedent.
4. **Theory revision.** While the current domain model may accurately account for all known observations, a new situation may be observed for which the model is inadequate.

PHINEAS, the current implementation of VBAL, uses Forbus' (1984, 1986) *Qualitative Process theory* to represent and reason about change in the physical world, and a modified version of Gentner's (1983) *Structure-Mapping theory* for analogical mapping. The system's primary analogy component, SME (Falkenhainer et al, 1986), is used to perform comparisons of similarity and map theories across domains. PHINEAS has been shown to discover a caloric theory of heat by analogy to liquid flow. It has also developed an explanation of oscillatory electrical circuits from its knowledge of mechanical oscillation.

1.2. Experimentation–Based Theory Revision: An Overview

Experimentation–based theory revision (Rajamoney, 1988) is an approach to changing or augmenting an incomplete or incorrect theory. Experimentation–based theory revision consists of three main steps:

1. **Contradiction detection.** Problems with the existing theory are detected by comparing the predictions based on the theory with the observations made from the real world. If the predictions and observations lead to a *contradiction* then the existing domain theory has to be revised.

[1] The term *analogue* is used in its most general sense throughout this paper. An analogy may be found within the same domain, as between one instance of liquid flow and another, or across domains, as between electron flow and liquid flow. No strong claims are made about the access mechanism, whose theoretical underpinnings are still under development. While implemented and autonomous, the accesser is far from sophisticated at this time.

2. **Hypothesis formation.** Hypotheses that involve changes to the existing theory are proposed. This stage is governed by *explanation construction* – only changes leading to a revised domain theory that can explain the observed phenomenon are proposed.
3. **Experiment design.** Typically, there will be a number of different ways to change a theory to explain a new phenomenon. Experiments are designed to identify the change that is consistent with the actual behavior of the real world (see Rajamoney, 1988). Hypotheses whose predictions are not consistent with experimental observations are rejected.

ADEPT is a system that demonstrates experimentation-based theory revision. It starts with an operational but initially incomplete and incorrect theory and revises it to conform to observations made from the real world. ADEPT has been demonstrated on a number of examples. It has successfully learned effects and conditions of physical processes such as a new influence of evaporation on the temperature of the evaporating liquid and a new condition for dissolving solutes requiring the concentration of the solution to be less than its saturation concentration.

2. An Integrated Model of Theory Development

Theory development is a dynamic process involving the formation of candidate theories, revisions to account for anomalous observations or achieve simplicity, and experimentation to test hypotheses and collect new data. These activities are highly interdependent yet highly modular. They may be performed by numerous people in distant locations, possibly across generations (e.g., the discourse between Copernicus, Galileo and Kepler, whose lives spanned nearly 200 years). In this section we develop this "collection of specialized experts" view of theory development with respect to theory formation, revision, and experimentation and show how the expertise of each is required to reduce the search space throughout the development cycle. We first describe strengths and limitations of our two methodologies and their complementary relationship. We then define a general protocol for interaction between systems specializing in theory formation, revision, and experimentation. Next, we show how the integrated system provides a comprehensive model for each stage of theory development.

2.1. Limitations and Strengths

As independent research efforts, each approach is designed to perform theory development autonomously. VBAL conjectures explanations of the new behavior based on its similarity to previously encountered phenomena. Its power lies in its ability to construct novel theories, focused by considering only theories for which it has an analogical precedent. However, VBAL has some important limitations. It is intended for passive observation and thus does not empirically test a hypothesis. It makes intermediate assumptions and depends on simulation experiments to test the consistency of these assumptions. This leads to questions about the validity of proposed theories. In addition, VBAL must rely on heuristics and prior experiences to guide search, thus requiring one to entertain hypotheses that might easily be empirically refuted.

In turn, experimentation-based theory revision locates known theories that appear relevant to the observation and modifies them to inclusively account for the new example. Its power lies in its ability to interact actively with the world, discriminate among alternative revisions, and refute proposed hypotheses. However, experimentation-based theory revision has some important

limitations. It is unable to make large, fundamental modifications to a theory, or produce one where none existed before. This limits it to revising "roughly correct" theories. Furthermore, experimentation is essentially open-ended in terms of what tests can be made and what kinds of experiments can be designed. For example, it may not be tractable to collect all possible hypotheses prior to conducting experiments.

The limitations of each approach corresponds nicely to the strengths of the other. Verification-based analogical learning provides:

1. Highly focused, theoretically motivated queries about the state of the world, such as checking for the existence of an anticipated object or testing theoretical predictions.
2. Large changes in theoretical perspective, develops new theories and provides candidate theories to revise.
3. A restricted number of potential hypotheses and a preferential ordering on hypotheses.

Experimentation-based theory revision provides:

1. Empirical tests for the relevance of certain perceived aspects of a situation, such as the necessity of ancillary processes normally associated with an analogue theory.
2. Discrimination among plausible hypotheses or refutation of a single hypothesis.
3. Experiments to detect the presence of an unnoticed or conjectured object or tests for conjectured properties of existing objects.
4. Probes of the situation for unknown values of a quantity or its derivatives.

2.2. A Communication Protocol

In this section we develop a general protocol for theory development tasks which enables one method to make use of another's expertise in a system independent manner. If the process answering a query lacks the appropriate decision procedure or is unable to successfully produce a response, a value of UNKNOWN is always acceptable. The protocol results in an extendible architecture, allowing new techniques to be added or existing techniques to be replaced by improved versions.

A crucial question concerns how one tells whether or not some fact holds. In theory formation and revision, we must assume incomplete knowledge. Thus, normal ways of deriving facts about the environment must be redefined. We distinguish between queries which depend primarily on the current beliefs of the system and queries which are able to question those beliefs by looking for alternate sources of information. *Direct queries* directly probe for the status of a condition using inference, or simple empirical tests if their status is not easily deducible. *Indirect queries* look for the effects normally associated with a condition, to test if deductive conclusions are wrong or if an analogous condition is in effect.

We decompose theory development into eight tasks, which suffice for a wide range of interesting problems:

Present? <object-or-variable> <primary-conditions> <secondary-conditions>
This queries for the existence of a partially specified, unknown object. Failure of any secondary conditions is not grounds for rejection, but may be used to reduce the set of candidates satisfying primary conditions. For example, investigation of a chemical reaction

may lead one to suspect and test for the presence of a particular catalyst in the mixture.

Test–Value <quantity> <value>
This instructs the system to search for an inferential determination of the quantity's value, or experimentally probe the situation for the value. The value may be left unspecified, or the truth of a particular relative value may be sought, as in (GREATER-THAN boiling-temperature) or DECREASING. For example, hypothesis generation may require the value of a quantity not reported in the initial observation.

Test–Condition <relation>
This determines if the specified relation holds. For example, investigation of heat–related theories may require determining if one object is in thermal contact with another.

Test–Effects <relation>
This is an indirect query which instructs the experimentation system to look for the presence of the known effects of a physical relation. For example, if Test-Condition had determined that a specified fluid path was not configured to support liquid flow, the validity of this conclusion may be questioned by looking for the effects of liquid flow through the path. Test-Effects may be used to seek an answer when Test-Condition returns unknown, instigate belief revision, or create a new concept analogous to the given physical relation.

Necessary? <condition> <observation>
The necessity of a condition thought to be essential to achieving an observation is questioned with this query. For example, a developing theory on chemical reactions may state that a particular catalyst is required. This query would call for experiments to determine if the catalyst is actually required.

Discriminate <hypotheses> <observation>
This asks the experiment design system to construct experiments to discriminate among a set of hypotheses that are thought to cause the observation. For example, during theory revision, several modifications of the original theory may explain the novel observation. This query finds those revisions that are consistent with information gathered from directed experiments.

Propose–Theories <*observation*>
This invokes the theory formation system to develop theories that will explain the observation. For example, during theory revision, experiments may rule out all the candidate revisions or the revision proposer may not find any consistent modifications to the theory. In such cases, the theory revision system uses this query to post a theory formation task.

Propose–Revisions <observation> <theory> <:condition or :effect>
This query asks the theory formation system, or a specialist in revision hypotheses, to propose revisions to a theory that will enable it to explain the observation. The query must specify if the revision should be to the theory's conditioning relations or to its set of effects.

2.3. The Three Stages to Developing a Complete and Consistent Theory

There are three primary stages to theory development within the VBAL framework: *Theory Generation*, *Theory Completion*, and *Theory Revision*. This section examines the interaction of the two systems in each of these stages and uses an implemented example to illustrate the interaction. The example involves forming and revising a model for *evaporation*. Throughout this section, we will assume that theories are represented by a set of *processes* and

individuals (objects) as defined in Forbus' (1984) Qualitative Process theory. Each process specifies a set of participatory *individuals* (objects and other processes), a set of *conditioning relations* indicating when it is active, and a set of *effects* that apply when it is active.

In our implementation of this integrated architecture, PHINEAS initiates the process of explaining new observations and posts tasks for ADEPT when its expertise is required. If an observation cannot be explained by existing theories, PHINEAS attempts to generate an explanation by recalling past observations of similar or analogous behavior. The knowledge used to explain these previous observations is used to analogously explain the current situation. In constructing the explanation, PHINEAS may call on ADEPT to measure the value of a quantity or determine the existence of a hypothesized object. In addition, experimentation and possible revision of the initial hypothesis may then be required for this or future observations. PHINEAS and ADEPT use the protocol to interactively solve such problems during theory formation and revision.

2.3.1. Theory Generation

Theory generation is the process of proposing an initial theory to explain a novel phenomenon. There are two stages to theory generation in VBAL. The first stage examines the current behavior and recalls previously understood similar behavior. Theories used to explain an analogue behavior are then mapped into the current domain and proposed as an initial explanation of the current phenomenon.

The system next divides the elements of each hypothesized theory into *primary processes* and *ancillary processes*. A primary process is one that affects an observed quantity, such as the temperature of an object whose temperature was observed. Ancillary processes are those that were used in explaining the analogue case, but do not directly affect one of the current observables. The necessity of a primary process is assumed and never experimentally questioned. Ancillary processes are eliminated during theory formation if they are found to be unnecessary.

The second stage in theory generation is to make the proposed explanations operational. A model is non–operational if it calls for participatory objects and processes whose presence was not noticed during the initial observation. If their existence cannot be determined (at this time), their existence must be assumed or the proposal modified to not depend on them. Operationalization first consists of instantiating each primary process by examining its unknown individuals:

When the individual is an uninstantiated, ancillary process:
  Attempt to instantiate it.
  If not instantiable, test for NECESSARY?.
    If necessary, reclassify it as a primary process, otherwise remove it.
When the unknown individual is an entity:
  Test for PRESENT?
  If not, postulate its existence and store its known set of characteristics.

Any ancillary process that is experimentally determined to be irrelevant is deleted from the generated theory. Remaining ancillary processes must be instantiated, if they have not been already. However, if that instantiation calls for postulating the existence of an unknown entity,

(Necessary? <ancillary-process> <observation>) will be invoked first. If a later contradiction occurs, the ancillary processes should be the first to be questioned during revision.

The final step in producing a fully operational theory is to test the analogically proposed conditioning relations for validity under the current conditions. This is done using Test-Value and Test-Condition. Conditioning relations not known to be true in the current context are temporarily removed in order to obtain a fully operational theory and enable discrimination with competing theories. For surviving theories, an attempt is then made to replace these conditioning relations with analogous relations applicable to the current context.

2.3.1.1. Evaporation Example: Generating Initial Hypotheses

This section describes how the integrated implementation generates an initial model for evaporation. The system begins with knowledge of six processes - liquid flow, heat flow, dissolving, spring oscillation, boiling and heat replenishment (to constantly maintain the heat of a stove). It also has a database of physical observations fully explained by these processes. Suppose an open beaker containing alcohol is left on a table top for a day, during which time the amount of alcohol is observed to decrease. The problem is to propose an explanation for this observation, which, according to the system's existing knowledge, should never have happened.

Model Creation: At this point, no known, instantiable theory is able to even partially explain the loss of alcohol in the beaker. By examining its knowledge of "similar" behaviors, PHINEAS determines that the only known examples of a liquid leaving a container call for it to flow out or to boil away. Three ordered, initial hypotheses, based on overall behavioral similarity, are generated. The first calls for the alcohol to flow out, the second calls for it to vaporize, and a distant third calls for it to dissolve based on its gradual disappearance. The initial vaporization explanation is shown in Figure 1. It consists of one primary process - boiling, and two ancillary processes - heat flow and heat replenishment, which are believed to be required for boiling to take place.

Model Operationalization: The three models (based on flow, boiling, and dissolving) call for the presence of objects that were undetected in the initial observation. We focus first on operationalizing the vaporization explanation. This explanation requires the presence of two unknowns - alcohol vapor in the beaker and a heat source. PHINEAS first produces the query:

```
(Present?  ?STEAM1  ((Contained-Gas ?STEAM1)            ;primary conditions
                     (Container-of ?STEAM1 beaker)
                     (Substance-of ?STEAM1 alcohol))
                    ())                                 ;no secondary conditions
```

Notice that the query is very specific - the object is fully specified and all that remains is to test if it is there. Of course, even this test can be non-trivial. To answer the query, ADEPT first examines the known set of objects and finds that none satisfy the primary conditions. It then examines its database of experimentation techniques, and recalls that litmus paper changes color in the presence of alcohol and can be used to test for the hypothesized presence of alcohol vapor in the beaker. The litmus paper test is conducted, via instructions to the assumed human assistant (such as, "make the litmus paper touch the air inside the beaker"), and a positive result confirming the presence of alcohol vapor is obtained.

```
ACCESS: Found the following applicable to observation OBSERVATION-1
  BMAP(2-CONTAINER-LF,OBSERVATION-1)
  BMAP(BOILING-PROTOTYPE,OBSERVATION-1)
  BMAP(SALT-DISSOLVING,OBSERVATION-1)
 . . .
(B-EXPLAINS
 (SET (PROCESS-DEFINITION PI1        ;derived from heat flow. An ancillary process.
        (IMPLIES
         (AND (INDIVIDUAL ?STOVE (CONDITIONS (QUANTITY (HEAT ?STOVE))))
              (INDIVIDUAL ALCOHOL1 (CONDITIONS (QUANTITY (HEAT ALCOHOL1))))
              (INDIVIDUAL BEAKER1 (CONDITIONS (HEAT-PATH BEAKER1)
                                              (HEAT-CONNECTION BEAKER1 ?STOVE ALCOHOL1)))
              (HEAT-ALIGNED BEAKER1)
              (GREATER-THAN (A (TEMPERATURE ?STOVE)) (A (TEMPERATURE ALCOHOL1))))
         (AND (QUANTITY (HEAT-FLOW-RATE PI1))
              (Q= (HEAT-FLOW-RATE PI1) (- (TEMPERATURE ?STOVE) (TEMPERATURE ALCOHOL1)))
              (I+ (HEAT ALCOHOL1) (A (HEAT-FLOW-RATE PI1)))
              (I- (HEAT ?STOVE) (A (HEAT-FLOW-RATE PI1))))))
       (PROCESS-DEFINITION PI2       ;derived from boiling. The primary process.
        (IMPLIES
         (AND (INDIVIDUAL ALCOHOL (CONDITIONS (SUBSTANCE ALCOHOL)))
              (INDIVIDUAL BEAKER1 (CONDITIONS (CAN-CONTAIN BEAKER1 ALCOHOL)))
              (INDIVIDUAL ALCOHOL1 (CONDITIONS (CONTAINED-LIQUID ALCOHOL1)
                                               (CONTAINER-OF ALCOHOL1 BEAKER1)
                                               (SUBSTANCE-OF ALCOHOL1 ALCHOHOL)))
              (INDIVIDUAL ?STEAM1 (CONDITIONS (CONTAINED-GAS ?STEAM1)
                                              (CONTAINER-OF ?STEAM1 BEAKER1)
                                              (SUBSTANCE-OF ?STEAM1 ALCHOHOL)))
              (INDIVIDUAL PI1 (CONDITIONS (PROCESS-INSTANCE HEAT-FLOW PI1)
                                          (DESTINATION PI1 ALCOHOL1)))
              (ACTIVE PI1)
              (NOT (LESS-THAN (A (TEMPERATURE ALCOHOL1)) (A (TBOIL ALCOHOL1))))
              (GREATER-THAN (A (AMOUNT-OF ALCOHOL1)) ZERO))
         (AND (QUANTITY (VAPORIZATION-RATE PI2))
              (Q= (VAPORIZATION-RATE PI2) (HEAT-FLOW-RATE PI1))
              (GREATER-THAN (A (VAPORIZATION-RATE PI2)) ZERO)
              (I- (HEAT ALCOHOL1) (A (VAPORIZATION-RATE PI2)))
              (I- (AMOUNT-OF ALCOHOL1) (A (VAPORIZATION-RATE PI2)))
              (I+ (AMOUNT-OF ?STEAM1)) (A (VAPORIZATION-RATE PI2)))))
       (PROCESS-DEFINITION PI3       ;derived from heat replenishment. An ancillary process.
        (IMPLIES
         (AND (INDIVIDUAL ?STOVE (CONDITIONS (HEAT-SOURCE ?STOVE)))
              (INDIVIDUAL PI1 (CONDITIONS (PROCESS-INSTANCE HEAT-FLOW PI1) (SOURCE PI1 ?STOVE)))
              (ACTIVE PI1))
         (AND (EQUAL-TO (D (HEAT ?STOVE)) ZERO)
              (I+ (HEAT ?STOVE) (A (HEAT-FLOW-RATE PI1)))))))
  OBSERVATION-1)
```

Figure 1: Creating an initial explanation of the evaporation observation. Here, PHINEAS hypothesizes, via behavioral analogy, that the set of three boiling-related processes explains the evaporation observation. At this stage, these processes are non-operational.

PHINEAS next produces a **Present?** query for the heat source. In this case, ADEPT returns a value of unknown: unable to deductively locate such an object or experimentally test for one. PHINEAS responds with

```
(Necessary? PI1 OBSERVATION-1)
```

which asks if the ancillary process PI1 (heat flow) is necessary to produce the observation. ADEPT proposes to repeat the observation, only this time thermally isolating the alcohol from potential heat flows by using an insulated container. When the amount of alcohol still decreases, the need for an external supply of heat is removed since it must be irrelevant to a potential explanation.

At this point, the vaporization explanation is fully instantiated and consists of a single, vaporization process. To make it fully operational, PHINEAS concludes with the following two queries about its proposed conditioning relations:

```
(Test-Value  (A (Temperature alcohol1))  ¬(Less-Than (A (TBoil alcohol1))))
(Test-Value  (A (Amount-of alcohol1))  (Greater-Than zero))
```

ADEPT determines that the first condition is false and the second is true. PHINEAS then deletes the first condition and retains the second condition in the vaporization model.[2] At this stage, the newly-formed vaporization model is completely instantiated, operational, and can fully explain the observed decrease in the amount of alcohol in the beaker.

The experimentally determined answers to these theoretically-motivated questions enabled the system to (1) confirm that alcohol vapor is present, (2) find that no known heat source exists, (3) determine that the type of heat flow associated with boiling is not a necessary component of the newly generated model of evaporation and (4) find that the boiling temperature is not required for the new process. A new *evaporation* model is conjectured as the explanation. The alternative derived from liquid flow is rejected due to the need to hypothesize the existence of unobservable entities (e.g., a destination liquid), which was not required of the evaporation model (i.e., Occam's razor).[3]

2.3.2. Theory Completion

Once an operational model has been produced, it must be tested for consistency with the observed behavior by using it to *envision* (Forbus, 1984) the possible behaviors of the current physical configuration. This corresponds to asking the question "what are the consequences of assuming this new theory?" Simulation may produce unanticipated theoretical predictions or uncover unanticipated interactions with existing theories (Falkenhainer, 1987). Experimentally testing theoretical predictions enables the system to refute a given hypothesis or strengthen its credibility. When unanticipated interactions among theories nullify the anticipated consequences of a hypothesized model, these interactions must be analyzed and theories revised.

At the close of theory completion, a (potentially empty) set of hypothesized models exists that completely and consistently explain the observed behavior. If more than one hypothesis is produced, the DISCRIMINATE task is used to eliminate those that can be experimentally refuted.

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[2] At model selection time, the attempt to restore the temperature condition fails when no analogous condition can be found.

[3] Once the need arose to hypothesize unseen entities, PHINEAS's agenda mechanism temporarily abandoned the liquid flow approach in favor of the boiling approach. The success of the boiling approach caused the system to permanently abandon the partially complete liquid flow hypothesis. Being third in preference, the dissolving hypothesis was never examined.

2.3.2.1. Evaporation Example: Completing the Theory Formation Process

The operational vaporization hypothesis contains the following three influences:

```
(I- (Heat alcohol1) (A (Vaporization-Rate PI2)))
(I- (Amount-of alcohol1) (A (Vaporization-Rate PI2)))
(I+ (Amount-of alcohol-vapor1) (A (Vaporization-Rate PI2)))
```

The influences on amount are consistent with the initial observation that the amount of alcohol liquid decreased. However, when this model is used to anticipate what will happen to a beaker of alcohol left sitting on a table, it produces two secondary predictions – the alcohol's temperature will drop, due to the loss of latent heat during vaporization, and the amount of vapor will increase. Since the alcohol's temperature across time was not originally reported, `Test-Value` is invoked for the anticipated change in temperature. ADEPT calls for the physical scenario to be repeated and changes in alcohol temperature noted. This test confirms the evaporation theory's hypothesis and verifies it as a complete and consistent explanation for the observed phenomenon.

2.3.3. Theory Revision

Theory revision occurs when an anomalous observation violates an existing model. The first step to revising an imperfect theory is blame assignment, which is done in a layered manner. First, hypotheses are made to determine if the contradiction is due to a process being incorrectly active or inactive, or if a process has an inappropriate causal effect. Once candidate processes have been identified, specific revision hypotheses are generated to modify either the process' conditions or its causal effects. Experimentation is used at each stage to eliminate refutable hypotheses. Experiments are proposed until the correct revision to the theory is found or until all hypotheses have been eliminated. This last case calls for a new round of theory formation.

2.3.3.1. Evaporation Example: Accounting for New Anomalous Observations

The newly formed theory of evaporation predicts that it will always be active as long as there is liquid in a container. When this theory is used to explain a second example of evaporation – evaporation in a closed container – a contradiction is detected when the amount of liquid stops decreasing after only a little liquid has disappeared. Since the system recognizes this as an instance of evaporation (which stopped too soon), ADEPT is invoked to revise the current model. It first determines experimentally that the problem is due to a failed conditioning relation rather than a failed effect relation. It thus queries PHINEAS (using `PROPOSE-REVISIONS`) for a set of candidate conditioning revisions. PHINEAS again recalls liquid flow and dissolving, due to their behavioral similarity and on the grounds that they were both observed to stop after being active for some time (i.e., the relevant problem with evaporation). Through analogous explanations for stopping, it proposes two new candidate quantity conditions – the amount of liquid has to be greater than the amount of vapor (from liquid flow) or the amount of vapor has to be less than some saturation point for the vapor (from dissolving). ADEPT experimentally refutes the first (by constructing an experiment to increase the amount of liquid and observing that evaporation does not start again) and finds the second to be consistent with experiments. This new saturation quantity condition is added to the evaporation model, yielding a theory consistent with existing experiences (Figure 2).

```
(PROCESS-3318
     Individuals  ((?V-3309 (Substance ?V-3309))
                   (?V-3310 (Can-Contain ?V-3310 ?V-3309))
                   (?V-3311 (Contained-Liquid ?V-3311)
                            (Container-of ?V-3311 ?V-3310)
                            (Substance-of ?V-3311 ?V-3309))
                   (?V-3312 (Contained-Gas ?V-3312)
                            (Container-of ?V-3312 ?V-3310)
                            (Substance-of ?V-3312 ?V-3309)))
     QuantityConditions  ((Greater-Than (A (Amount-of ?V-3311)) zero)
                          (Less-Than (A (Amount-of ?V-3312)) (A (Saturation-3326 ?V-3312))))
     Relations  ((Quantity (Vaporization-Rate ?self))
                 (Greater-Than (A (Vaporization-Rate ?self)) zero))
     Influences ((I- (Heat ?V-3311) (A (Vaporization-Rate ?self)))
                 (I- (Amount-of ?V-3311) (A (Vaporization-Rate ?self)))
                 (I+ (Amount-of ?V-3312) (A (Vaporization-Rate ?self)))))
```

Figure 2: The hypothesized model of evaporation in its final, revised form.

3. An Additional Example: Understanding Osmosis

Consider a case of forming and revising a model for *osmosis*. In this example, the system is shown two containers separated by a partition which, unknown to the system, is semi-permeable (Figure 3). It observes the amount of solution decreasing in one container and increasing in the other. The system is unable to explain these observations since none of the known processes are active. A number of processes are candidates for revision: absorption, boiling, condensation, evaporation, or flow. However, due to its ability to detect behavioral similarity, the system focuses first on liquid flow. Using the `Present?` query, it finds two potential paths for a flow: the membrane separating the two solutions and the wall of their shared container. PHINEAS then finds, using `Test-Condition`, that neither object is `Fluid-Aligned` (able to transport fluids), since they are solid objects. It temporarily removes this precondition to form two operational, competing theories. ADEPT, in response to a `Discriminate` task, experimentally rules out flow through the container wall while all experiments continue to substantiate the membrane hypothesis. Now that it has a complete and consistent theory, PHINEAS looks for an analogue to the `Fluid-Aligned` precondition. After positively testing for the effects of the more general *aligned* concept, PHINEAS hypothesizes an analogue to `Fluid-Aligned` (called `Aligned-3417`), which ADEPT determines is a function of the membrane substance. The dependency of osmosis on concentration may then be determined during revision to accommodate future observations (as in Rajamoney, 1986).

4. Evidence from the History of Science and Psychology

History is filled with examples of analogy being used for hypothesis generation. followed by systematic analysis and experimentation (e.g., Oppenheimer, 1956; Dreistadt, 1968; Gentner & Jeziorski, 1987). For example, Black's theories of latent heats of vaporization were developed by analogy with previously theories of melting. A year later, when a steady heat source was available, he conducted quantitative experiments (Roller, 1961). One particularly clear example

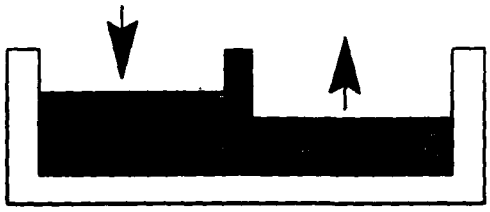

Figure 3: Osmosis example. The solution level in the left chamber is decreasing, while the solution in the right chamber is increasing.

of analogical hypothesis generation appears in Carnot's use of an elaborate analogy between water–driven and heat–driven engines in his development of the Carnot cycle:

> In the waterfall the motive power is exactly proportional to the difference of level between the higher and lower reservoirs. In the fall of caloric the motive power undoubtedly increases with the difference of temperature between the warm and the cold bodies; but we do not know whether it is proportional to this difference... It is a question which we propose to examine hereafter. (Carnot, 1977, page 15)

This hypothesis was later experimentally verified and may now be derived from the first law of thermodynamics. While Carnot assumed the caloric theory, the Carnot cycle and Carnot principle laid the foundations for the second law of thermodynamics, which is independent of caloric or mechanical theories of heat. The psychological literature also includes numerous studies of people using analogy to hypothesize solutions to problems or explanations of physical behavior. Construction of mental or physical experiments is a commonly observed post–hypothesis behavior (e.g., Clement, 1986; Collins & Gentner, 1987).

5. Related Work

Unlike the data–driven, weak methods of traditional systems in machine discovery such as BACON, STAHL, DALTON (Langley et al, 1981, 1987) and ABACUS (Falkenhainer et al, 1986), our system is theory–driven and knowledge–intensive. More closely related to our integrated model of theory formation, revision, and experimentation are Dietterich and Buchanan's (1983) EG and Shrager's (1987) IE. EG stressed the need for experimentation in theory formation and focused on how experimentation could constrain a potentially unwieldy hypothesis generator. While we incorporate this aspect, we also emphasize the important role that a highly focused theory generator may have on experimentation. In IE, the central claim is that careful causal analysis is unnecessary for tasks such as forming simple models of complex devices. Our primary concern is scientific theory formation which calls for a more methodical approach. though it seems that our design could apply to understanding everyday devices. Our work also shares some similarities with the IDS system (Nordhausen & Langley, 1987), which uses experimentation to induce qualitative models. Unlike IDS, our system uses analogy to focus the formation and revision of theories, and directed experiments to test the generated and revised theories.

6. Discussion

Here we have explored the strengths of combining two distinct theory formation and revision systems to form an integrated system based on analogy and experimentation. We showed how such an integration results in a more complete account of the entire scientific discovery process. Theory formation, revision and experimentation are viewed as interrelated and interdependent processes that require each system to postulate well-defined, theoretically motivated queries to use the expertise of the other.

The evaporation example illustrates many finer points of the discovery process. In the evaporation example, a person typically wouldn't generate all possible hypotheses (e.g., evaporation, liquid flow, absorption, vanish, invisible, etc.) and then discriminate between them. The space of hypotheses is made tractable by pruning based on a knowledge of what can happen *and* a knowledge of what is likely to happen (based on analogical precedents). Also, the presence of an experiment generator enabled us to test for the presence of alcohol vapor, rather than having to assume its existence and expend effort on a potentially incorrect hypothesis.

We are still far from programs that truly reflect actual scientific discovery processes. For example, we are strongly bounded by the complexity of qualitative reasoning and must limit explorations to discovering overly simplistic theories. Furthermore, the knowledge bases and reasoning sophistication of existing discovery systems are far too small to escape the "discovering Newton's laws in a day" phenomenon. However, this work takes steps towards realizing the scale and flavor of the task. Furthermore, it has made limitations in the systems clearer and provides a catalyst for further development. Future research in this direction involves modeling an entire cycle of scientific discovery using an example from the history of science such as the formation, revision and, finally, rejection of the caloric theory of heat.

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This work has benefited significantly from discussions with Gerald DeJong, Ken Forbus, Dedre Gentner, and John Collins. This research is supported in part by an IBM Graduate Fellowship to Falkenhainer, by a University of Illinois Cognitive Science / Artificial Intelligence Fellowship to Rajamoney, and by the Office of Naval Research under grants N00014-85-K-0559 and N00014-86-K-0309.

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Unita di ricerca di
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Dr. William M. Bart
University of Minnesota
Dept. of Educ. Psychology
330 Burton Hall
178 Pillsbury Dr., S.E.
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Department of Computer Science
Box 1688, Station B
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Teachers College, Box 8
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Center for the Study of Reading
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51 Gerty Drive
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XEROX Palo Alto Research
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3333 Coyote Road
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James S. McDonnell Foundation
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Center for the Study of Reading
University of Illinois
51 Gerty Drive
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1718 Connecticut Ave., N.W.
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Box 11A, Yale Station
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Princeton, NJ 08541

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Applications Division
Admiralty Research Establishment
Portsdown, Portsmouth PO6 4AA
UNITED KINGDOM

Dr. Dedre Gentner
University of Illinois
Department of Psychology
603 E. Daniel St.
Champaign, IL 61820

Chair, Department of
Psychology
Georgetown University
Washington, DC 20057

Dr. Robert Glaser
Learning Research
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University of Pittsburgh
3939 O'Hara Street
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Elliott Hall
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228 Uris Hall
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IBM T. J. Watson Research Ctr.
P.O. Box 704
Yorktown Heights, NY 10598

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University of California
Department of Information
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Irvine, CA 92717

Dr. David Kieras
Technical Communication Program
TIDAL Bldg., 2360 Bonisteel Blvd.
University of Michigan
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Orlando Field Unit
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University of Colorado
Boulder, CO 80309-0345

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Carnegie-Mellon University
Department of Psychology
Schenley Park
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Georgia Institute of Technology
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Columbia University
406 Schermerhorn Hall
New York, NY 10027

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University of Texas at Austin
Department of Computer Sciences
Taylor Hall 2.124
Austin, Texas 78712

Dr. David R. Lambert
Naval Ocean Systems Center
Code 772
271 Catalina Boulevard
San Diego, CA 92152-5000

Dr. Pat Langley
University of California
Department of Information
and Computer Science
Irvine, CA 92717

Dr. Marcy Lansman
University of North Carolina
The L. L. Thurstone Lab.
Davie Hall CB #3270
Chapel Hill, NC 27514

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Carnegie-Mellon University
Department of Psychology
Pittsburgh, PA 15213

Dr. Jean Lave
Institute for Research
on Learning
3333 Coyote Hill Road
Palo Alto, CA 92304

Dr. Robert W. Lawler
Matthews 118
Purdue University
West Lafayette, IN 47907

Dr. Alan M. Lesgold
Learning R&D Center
University of Pittsburgh
Pittsburgh, PA 15260

Dr. Jim Levin
Department of
Educational Psychology
210 Education Building
1310 South Sixth Street
Champaign, IL 61820-6990

Dr. John Levine
Learning R&D Center
University of Pittsburgh
Pittsburgh, PA 15260

Dr. Michael Levine
Educational Psychology
210 Education Bldg.
University of Illinois
Champaign, IL 61801

Dr. Clayton Lewis
University of Colorado
Department of Computer Science
Campus Box 430
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NETPMSA
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Naval Center for Applied Research
in Artificial Intelligence
Naval Research Laboratory
Code 5510
Washington, DC 20375-5000

Dr. Sandra P. Marshall
Dept. of Psychology
San Diego State University
San Diego, CA 92182

Dr. Manton M. Matthews
Department of Computer Science
University of South Carolina
Columbia, SC 29208

Dr. Richard E. Mayer
Department of Psychology
University of California
Santa Barbara, CA 93106

Dr. Joseph C. McLachlan
Code 52
Navy Personnel R&D Center
San Diego, CA 92152-6800

Dr. James McMichael
Technical Director
Navy Personnel R&D Center
San Diego, CA 92152-6800

Dr. Barbara Means
SRI International
333 Ravenswood Avenue
Menlo Park, CA 94025

Dr. Douglas L. Medin
Department of Psychology
University of Illinois
603 E. Daniel Street
Champaign, IL 61820

Dr. George A. Miller
Dept. of Psychology
Green Hall
Princeton University
Princeton, NJ 08540

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Behavioral Technology
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Chair, Department of
Computer Science
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Annapolis, MD 21402

Dr. Allen Newell
Department of Psychology
Carnegie-Mellon University
Schenley Park
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University of Michigan
Institute for Social Research
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Dr. A. F. Norcio
Code 5530
Naval Research Laboratory
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C-015
Institute for Cognitive Science
University of California
La Jolla, CA 92093

Deputy Technical Director
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San Diego, CA 92152-6800

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San Diego, CA 92152-6800

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San Diego, CA 92152-6800

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Code 2627
Washington, DC 20390

Dr. Harold F. O'Neil, Jr.
School of Education - WPH 801
Department of Educational
Psychology & Technology
University of Southern California
Los Angeles, CA 90089-0031

Dr. Stellan Ohlsson
Learning R & D Center
University of Pittsburgh
Pittsburgh, PA 15260

Office of Naval Research
Code 1133
800 North Quincy Street
Arlington, VA 22217-5000

Office of Naval Research,
Code 1142
800 N. Quincy St.
Arlington, VA 22217-5000

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Arlington, VA 22217-5000

Psychologist
Office of Naval Research
Branch Office, London
Box 39
FPO New York, NY 09510

Special Assistant for Marine
Corps Matters,
ONR Code 00MC
800 N. Quincy St.
Arlington, VA 22217-5000

Dr. Judith Orasanu
Basic Research Office
Army Research Institute
5001 Eisenhower Avenue
Alexandria, VA 22333

Dr. James Paulson
Department of Psychology
Portland State University
P.O. Box 751
Portland, OR 97207

Military Assistant for Training and
Personnel Technology,
OUSD (R & E)
Room 3D129, The Pentagon
Washington, DC 20301-3080

Dr. David N. Perkins
Project Zero
Harvard Graduate School
of Education
7 Appian Way
Cambridge, MA 02138

Dr. Nancy N. Perry
Naval Education and Training
Program Support Activity
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Pensacola, FL 32509-5000

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Twente University of Technology
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P.O. Box 217
7500 AE ENSCHEDE
THE NETHERLANDS

Dr. Steven E. Poltrock
MCC
3500 West Balcones Center Dr.
Austin, TX 78759-6509

Dr. Harry E. Pople
University of Pittsburgh
Decision Systems Laboratory
1360 Scaife Hall
Pittsburgh, PA 15261

Dr. Mary C. Potter
Department of Brain and
Cognitive Sciences
MIT (E-10-039)
Cambridge, MA 02139

Dr. Joseph Psotka
ATTN: PERI-IC
Army Research Institute
5001 Eisenhower Ave.
Alexandria, VA 22333-5600

Dr. Lynne Reder
Department of Psychology
Carnegie-Mellon University
Schenley Park
Pittsburgh, PA 15213

Dr. Steve Reder
Northwest Regional
Educational Laboratory
400 Lindsay Bldg.
710 S.W. Second Ave.
Portland, OR 97204

Dr. James A. Reggia
University of Maryland
School of Medicine
Department of Neurology
22 South Greene Street
Baltimore, MD 21201

Dr. J. Wesley Regian
AFHRL/IDI
Brooks AFB, TX 78235

Dr. Fred Reif
Physics Department
University of California
Berkeley, CA 94720

Dr. Lauren Resnick
Learning R & D Center
University of Pittsburgh
3939 O'Hara Street
Pittsburgh, PA 15213

Dr. Gilbert Ricard
Mail Stop K02-14
Grumman Aircraft Systems
Bethpage, NY 11787

Dr. Linda G. Roberts
Science, Education, and
Transportation Program
Office of Technology Assessment
Congress of the United States
Washington, DC 20510

Dr. William B. Rouse
Search Technology, Inc.
4725 Peachtree Corners Circle
Suite 200
Norcross, GA 30092

Dr. Roger Schank
Yale University
Computer Science Department
P.O. Box 2158
New Haven, CT 06520

Dr. Alan H. Schoenfeld
University of California
Department of Education
Berkeley, CA 94720

Dr. Janet W. Schofield
816 LRDC Building
University of Pittsburgh
3939 O'Hara Street
Pittsburgh, PA 15260

Dr. Judith W. Segal
OERI
555 New Jersey Ave., NW
Washington, DC 20208

Dr. Colleen M. Seifert
Institute for Cognitive Science
Mail Code C-015
University of California, San Diego
La Jolla, CA 92093

Dr. Ben Shneiderman
Dept. of Computer Science
University of Maryland
College Park, MD 20742

Dr. Lee S. Shulman
School of Education
507 Ceras
Stanford University
Stanford, CA 94305-3084

Dr. Robert S. Siegler
Carnegie-Mellon University
Department of Psychology
Schenley Park
Pittsburgh, PA 15213

Dr. Derek Sleeman
Computing Science Department
King's College
Old Aberdeen AB9 2UB
Scotland
UNITED KINGDOM

Dr. Richard E. Snow
School of Education
Stanford University
Stanford, CA 94305

Dr. Elliot Soloway
Yale University
Computer Science Department
P.O. Box 2158
New Haven, CT 06520

Distribution List [Illinois/Gentner] NR 667-551

Dr. Richard C. Sorensen
Navy Personnel R&D Center
San Diego, CA 92152-6800

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Brown University
Department of Psychology
Providence, RI 02912

Dr. Robert J. Sternberg
Department of Psychology
Yale University
Box 11A, Yale Station
New Haven, CT 06520

Dr. Thomas Sticht
Applied Behavioral and
Cognitive Sciences, Inc.
P.O. Box 6640
San Diego, CA 92106

Dr. John Tangney
AFOSR/NL, Bldg. 410
Bolling AFB, DC 20332-6448

Dr. Kikumi Tatsuoka
CERL
252 Engineering Research
Laboratory
103 S. Mathews Avenue
Urbana, IL 61801

Dr. Perry W. Thorndyke
FMC Corporation
Central Engineering Labs
1205 Coleman Avenue, Box 580
Santa Clara, CA 95052

Dr. Martin A. Tolcott
3001 Veasey Terr., N.W.
Apt. 1617
Washington, DC 20008

Dr. Douglas Towne
Behavioral Technology Labs
University of Southern California
1845 S. Elena Ave.
Redondo Beach, CA 90277

Chair, Department of
Computer Science
Towson State University
Towson, MD 21204

Headquarters, U. S. Marine Corps
Code MPI-20
Washington, DC 20380

Dr. Kurt Van Lehn
Department of Psychology
Carnegie-Mellon University
Schenley Park
Pittsburgh, PA 15213

Dr. Jerry Vogt
Navy Personnel R&D Center
Code 51
San Diego, CA 92152-6800

Dr. Beth Warren
BBN Laboratories, Inc.
10 Moulton Street
Cambridge, MA 02238

Dr. Keith T. Wescourt
FMC Corporation
Central Engineering Labs
1205 Coleman Ave., Box 580
Santa Clara, CA 95052

Dr. Douglas Wetzel
Code 51
Navy Personnel R&D Center
San Diego, CA 92152-6800

Dr. Barbara White
BBN Laboratories
10 Moulton Street
Cambridge, MA 02238

Dr. Robert A. Wisher
U.S. Army Institute for the
Behavioral and Social Sciences
5001 Eisenhower Avenue
Alexandria, VA 22333-5600

Dr. Martin F. Wiskoff
Defense Manpower Data Center
550 Camino El Estero
Suite 200
Monterey, CA 93943-3231

Mr. John H. Wolfe
Navy Personnel R&D Center
San Diego, CA 92152-6800

Dr. Wallace Wulfeck, III
Navy Personnel R&D Center
Code 51
San Diego, CA 92152-6800

Dr. Masoud Yazdani
Dept. of Computer Science
University of Exeter
Prince of Wales Road
Exeter EX44PT
ENGLAND

Mr. Carl York
System Development Foundation
1 Maritime Plaza, #1770
San Francisco, CA 94111

Dr. Joseph L. Young
National Science Foundation
Room 320
1800 G Street, N.W.
Washington, DC 20550