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*Evaluation of the Fundamental Research  
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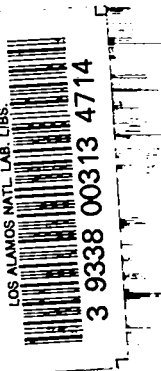
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## Evaluation of the Fundamental Research on Explosives (FRE) Program



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EVALUATION OF THE FUNDAMENTAL RESEARCH  
ON EXPLOSIVES (FRE) PROGRAM

by

Thomas Rivera and Ronald L. Rabie

ABSTRACT

A means to quantify both progress and the relative importance of the various tasks composing a large research program is discussed. The discussion is within the context of the particular example of the Fundamental Research on Explosives (FRE) program currently at the Los Alamos National Laboratory. The analysis reveals a strong connection in the generally parallel layout of the FRE program to planning for crisis aversion. The analysis is found to be valuable in obtaining a view of an existing R&D program in terms of its current probability of meeting its goals.

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I. INTRODUCTION

The task of formulating and managing basic R&D can bring about a time of serious trial for management and scientists involved in the research. Issues such as micromanagement of research and freedom to pursue serendipitous results not on the main track of the program can become monumental stumbling blocks in the path of progress. Indeed, the very definition of progress can occupy hours of management and technical-staff time. Such observations have led managers of basic technical-research programs to try numerous means for evaluating either the worthiness of a proposed program or the progress of a program already identified as worthy. We discuss, in the context of a particular example, a means to quantify both progress and relative importance of the various tasks composing a large basic research program. The approach we take is an extension of a technique proposed by Philip A. Roussel in an article in the Harvard Business Review titled "Cutting Down the Guesswork in R&D."<sup>1</sup>

The test case is a current program of basic research at the Los Alamos National Laboratory directed toward the accomplishment of a stated goal. The

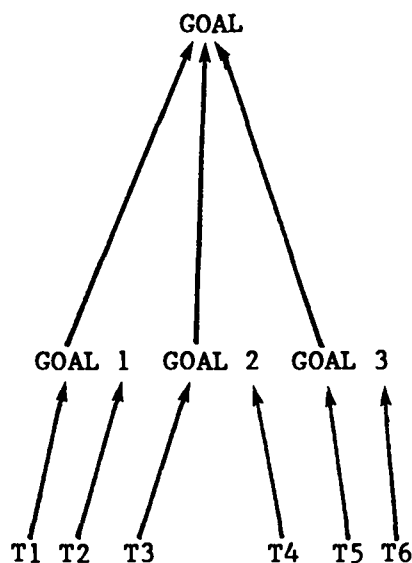
goal of this research is to obtain a detailed molecular-level understanding of the process of energy transfer among and within explosive molecules that results in the ability of explosives to sustain detonation. No such understanding currently exists, and we deem such a research program to be valuable to our long-term interest in the use of explosives at the Laboratory. This research activity is called the Fundamental Research on Explosives (FRE) program and is funded at a level of \$2.1 million during the current fiscal year (1984). This program has enjoyed similar levels of funding during the past two years, and we anticipate this level of funding to continue through fiscal 1985. The FRE program requires the research activities of more than 20 scientists in traditionally diverse areas. In fact, these individuals reside in three directorates (a directorate may contain 2,000 people). These directorates are variously responsible for physics and mathematics, chemistry, and engineering sciences. Funding for this program derives from all three directorates, and all three have a great interest in the progress of this research.

The size and diversity of the FRE program result in a certain difficulty for management. No single person is likely to have all the requisite technical knowledge needed to make unerring decisions on starting new initiatives and terminating unproductive avenues of inquiry. In fact, just the use of the word "unproductive" in reference to some task is likely to spark lengthy and heated debate. Nevertheless, all the parties involved in the program need to understand what constitutes progress and, further, to understand that management decisions made on behalf of the program are not capricious, but are based on an understandable method of assessing the value of a task to the accomplishment of the goals of the program. This last observation is the principal reason for seeking a definitive, workable, and understandable methodology for the evaluation of progress.

## II. THE EVALUATION PROCEDURE

Roussel directed his attention to a problem we will refer to as serial. In a serial problem, one assigns a probability of success to each element of the series. The series might be schematically represented as TASK 1  $\rightarrow$  TASK 2  $\rightarrow$  TASK 3  $\rightarrow$  ...  $\rightarrow$  GOAL. In such a serial example, one assigns probabilities

of success to each task and forms the product of the assigned probabilities to obtain the likelihood of achieving the goal. The management/technical-research staff interaction is composed of assigning the probabilities to the tasks. Management generally makes the final funding decision on the basis of how the probability of achieving the goal stacks up against potential losses that might be incurred if the goal is attained by the competition. Roussel's article was actually a bit less restrictive than the very simple serial case just presented but was not characteristic of the problem we face with the FRE program. The FRE program is more parallel in structure than serial. Schematically, the FRE looks more like a pyramid.



The various tasks being performed feed the intermediate goals and these intermediate goals feed the final goal. The first thing that becomes evident in such a structure is that one could accomplish only parts of the elemental tasks and still learn enough from them to result in a nearly complete attainment of one of the intermediate goals. In fact, it is just such an observation that encourages a manager to establish a parallel research structure. The likelihood of success is increased by introducing tasks that, at first glance, may appear to be redundant. Evaluating such a structure with respect to critical paths and probabilities of success is more involved than the simple serial

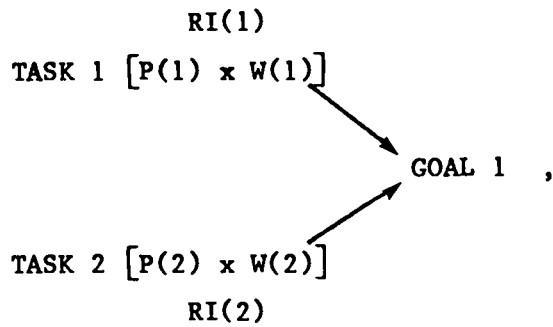
case. We have found that the evaluation of pyramid-like structures involves both the assignment of probabilities (done by the researchers) and the assignment of weights based on input from the researchers but done by the management. The probabilities represent the best estimates of the research staff as to the likelihood of accomplishment of the tasks within the time frame allowed. The weights are a measure of the importance of the tasks to accomplishment of the intermediate and final goals. The probabilities and weights are dynamic quantities that must be adjusted throughout a program's life. The combination of these quantities provides both the research staff and the technical management with a means for evaluating "critical paths" through complex programs as well as evaluating progress toward a program goal.

Before proceeding to a detailed example, we think it is important to distinguish between research done to further the knowledge of mankind and research done toward an end product or a specific goal. In the case of basic research done exclusively for academic satisfaction, the researcher must be as free as possible to pursue any avenue open to him. Interesting side issues and curiosities are the stuff of which general scientific advances are made. Such research is generally managed by the researcher, with time and cleverness being the only management issues. However, research performed in pursuit of a specific goal or an end product is usually a large collaborative effort, and the freedom to pursue all avenues becomes restricted. A great part of our success will depend on informing all participants regularly, in detail, of the status of the program. Knowledge of a problem is a large part of the solution.

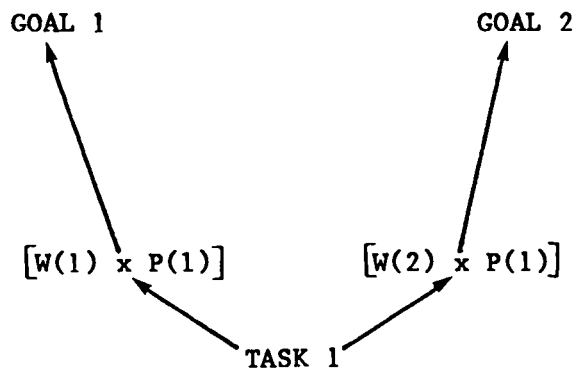
### III. EVALUATION OF THE FRE

#### A. Definition of Terms

We define the probability of accomplishing the  $i$ th task to be  $P(i)$  and the weight or figure of merit associated with that task to be  $W(i)$ . Figure of merit represents that portion of a stated goal that can possibly be accomplished assuming ideal conditions exist. Figures of merit are normalized so that the sum of the normalized figures of merit is equal to unity. The analysis is composed of a primitive-element analysis for a parallel element. This element may be represented as



where the normalized figures of merit and probabilities are multiplied to form what we call a relative importance product  $RI(i)$ . The sum of  $RI(1)$  and  $RI(2)$  is taken as the probability of accomplishing GOAL 1. This sum represents a "worst-case" situation in which no synergistic effects among the various tasks are taken into account. Therefore, this figure is a minimum probability ("or" probability) figure for success. This procedure is independent of the number of parallel tasks feeding a goal. It is very important to recognize that a particular task may acquire a large  $RI$  only by being comparatively probable and comparatively important. This fact allows the easy determination of "critical paths" once assignments of  $P(i)$  and  $W(i)$  are made. "Critical paths" in this context are shown in the example below. One should also recognize that a single task may be important to more than one goal. In such cases, the probability of accomplishing the task is constant over the affected goals, but the weights assigned to the task will depend on the various goals. Thus, the  $RI$  for the task will vary, depending upon the goals affected. A simple example is shown below.





If we assume that  $W(1) = 0.9$  and  $W(2) = 0.1$  for  $P(1) = 0.8$ , we find that  $RI(1) = W(1) \times P(1) = 0.72$ , while  $RI(2) = W(2) \times P(1) = 0.08$ ; that is,  $RI(1) > RI(2)$  because  $W(1) > W(2)$ . Clearly, TASK 1 is far more important to the accomplishment of GOAL 1 than it is to the accomplishment of GOAL 2. In subsequent steps of the analysis, the accomplishment of GOAL 1 may be found to be more important to attainment of the final goal of the program than is the accomplishment of GOAL 2. The path from TASK 1 through GOAL 1 to the final goal is an example of a "critical path."

It is important to realize that the tasks being discussed in the mathematical formulation above are primitive elements (an example might be getting an oscilloscope record). The tasks to be discussed below are more complex. An effort has been made to simplify the picture, but it should be kept in mind that not all cross-interactions or synergistic effects have been taken into account.

#### B. FRE Approach

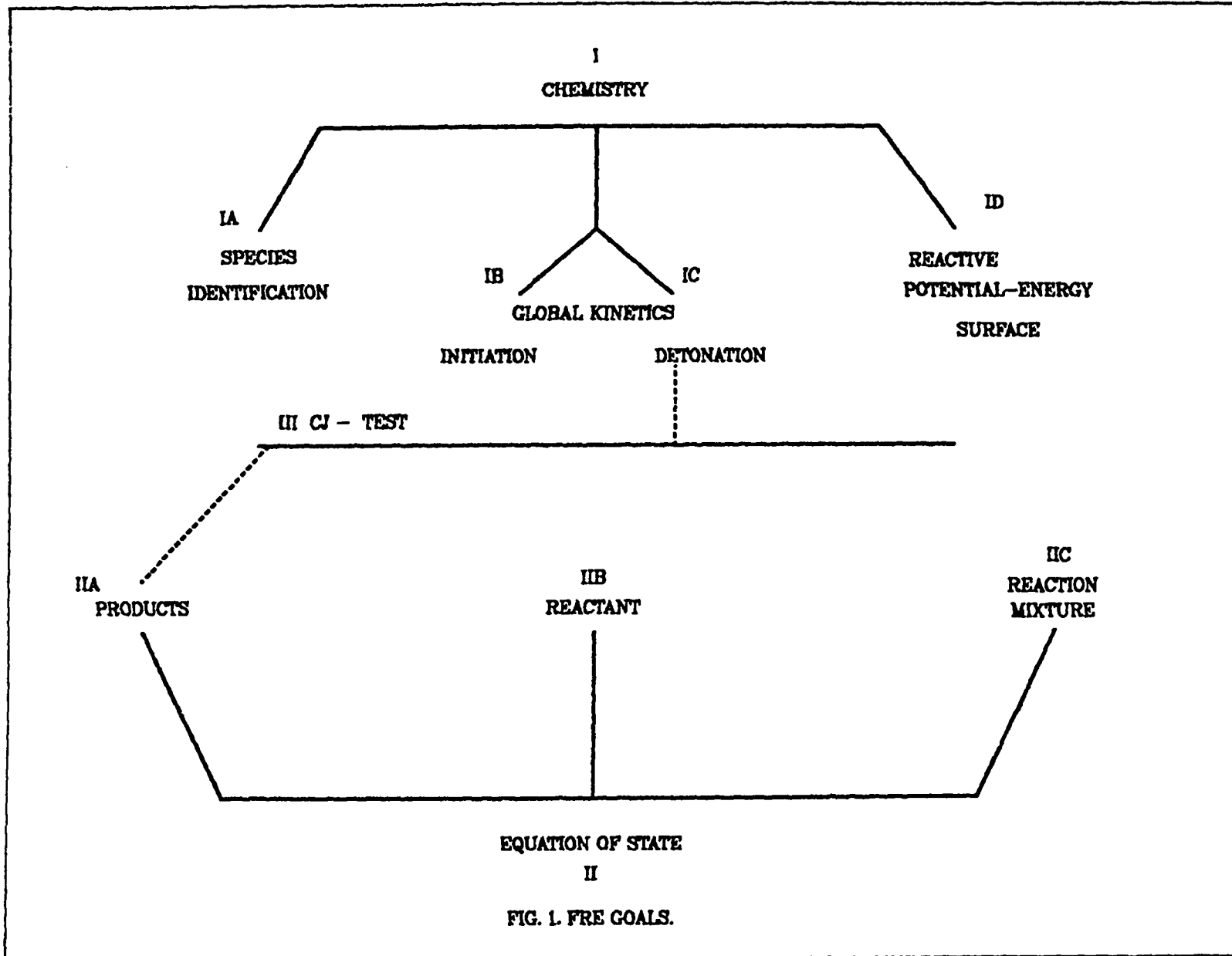
A team of scientific experts (the FRE Team) having the common interest of gaining the fundamental knowledge inherent in the program goals was assembled at the start of the FRE program. The various projects began as soon as a judicious choice of a simple-molecule prototype explosive, liquid nitric oxide, was made.

The accomplishment of individual tasks leading to acquisition of fundamental knowledge of the chemistry and equation of state of shocked or detonating liquid nitric oxide became the FRE approach. The FRE goals are outlined in Fig. 1.

The various tasks included in the effort were categorized into three areas: hydrodynamics (H), theory (T), and spectroscopy (S). The task titles grouped according to the three categories are summarized in Fig. 2. For simplicity, the notations given in Figs. 1 and 2 will be used in subsequent discussions. Figure 3 shows how the tasks and goals interconnect in achieving the final program goal. Because of the complex nature of the FRE program, the interconnecting lines shown in Fig. 3 represent the most significant interactions and do not represent all the interactions within the program nor any input from projects not funded through the FRE.

### C. Quantitative Assignments

Necessary conditions prior to the assignment of figures of merit and probabilities of success are 1) a definitive interpretation of what constitutes success for each task, and 2) a thorough understanding of the technical aspects of each project involved. A technical advisory committee (TAC), comprising technical experts in each of the three categories, was formed to assist the management in meeting these conditions. Based on the assumption that necessary conditions have been met, the quantitative assignments as presented below were made.



## HYDRODYNAMICS

- H1: Shocked-state measurements.
- H2: Detonation physics.
- H3: Shock-induced reaction histories.
- H4: Piston-cylinder measurements.

## THEORY

- T1: Dense-fluid thermodynamics.
- T2: Potential-energy surfaces.
- T3: Chemical dynamics.

## SPECTROSCOPY

- S1: Spectroscopy of shocked material.
- S2: Diamond cell spectroscopy.
- S3: Highly excited molecules and clusters.
- S4: Mass spectrometry of detonation products.
- S5: Elastic scattering.

Fig. 2. FRE Categories.

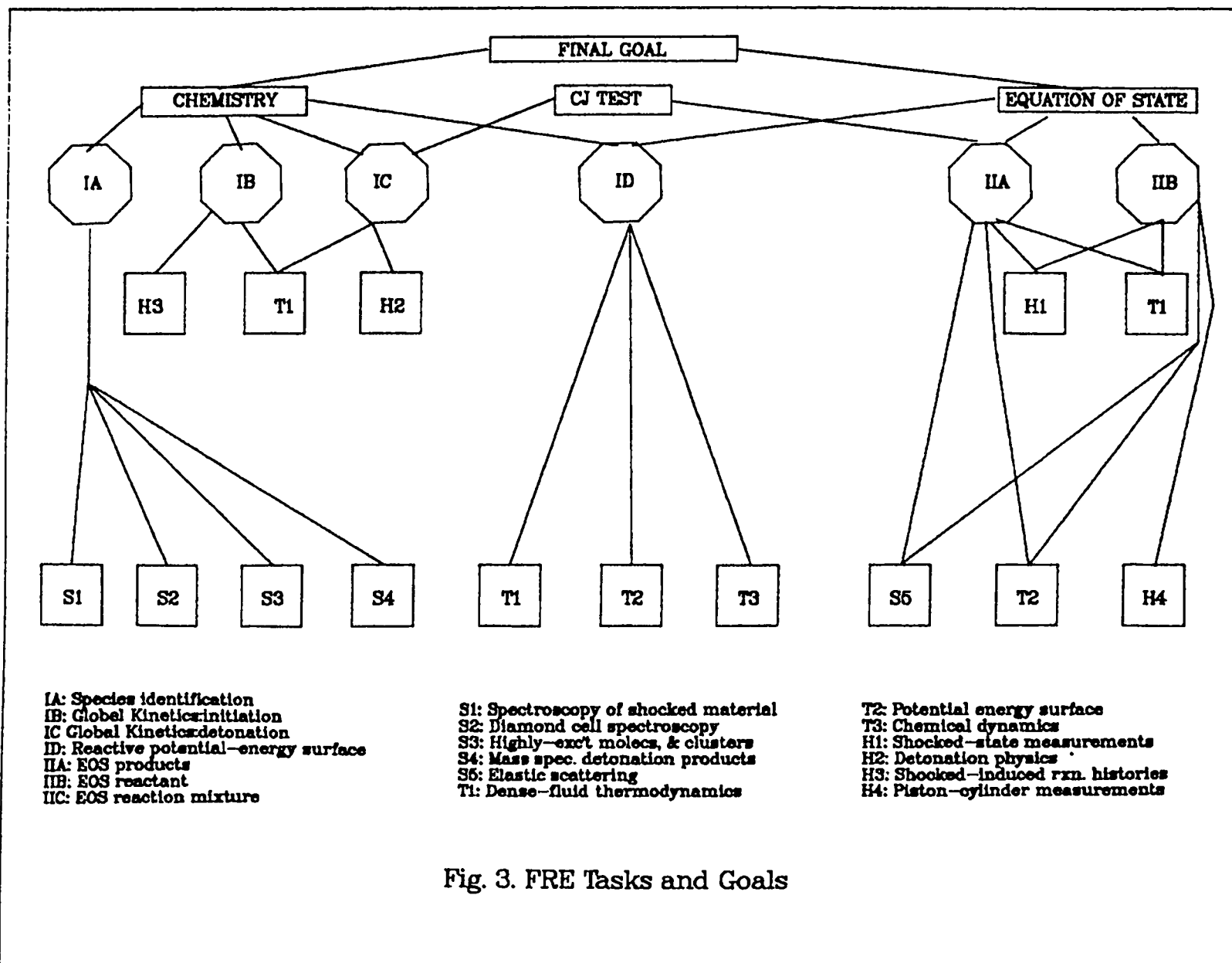


Fig. 3. FRE Tasks and Goals

#### IV. RESULTS

Each task (T) that leads to attaining a given subgoal (S) has assigned to it a figure of merit (M) as described above. This represents an estimate of the per cent of S that can be attained by T. Along with this, an estimate of the probability (P) for successful completion of task T is assigned.

All tasks having significant input to subgoal S are grouped together and normalized, such that

$$N \sum M(i) = W(i) \quad , \quad (1)$$

where N is a normalization constant.

Example - a specific example to illustrate this procedure is presented below

S = subgoal IA: Qualitative and quantitative identification of chemical species present in shocked and/or detonating liquid nitric oxide (NO).

T(1) = task S1: Coherent Raman spectroscopic interrogation of shock-compressed liquid NO.

$$M = 0.85 \quad P = 0.70$$

T(2) = task S2: Spectroscopic investigations of highly compressed NO in diamond-anvil cells.

$$M = 0.60 \quad P = 0.85$$

T(3) = task S3: Chemical-dynamics studies of highly excited species and molecular beam clusters of NO.

$$M = 0.55 \quad P = 0.55$$

T(4) = task S4: Chemical investigation of NO detonation products.

$$M = 0.60 \quad P = 0.60$$

A summary of figures of merit, probabilities, and relative importance for IA is presented in Table I.

TABLE I

## TASK RELATIVE IMPORTANCE FOR IA

<u>Subgoal</u>	<u>Task</u>	<u>M</u>	<u>W</u>	<u>P</u>	<u>RI</u>
IA	S1	0.85	0.33	0.70	0.23
	S2	0.60	0.23	0.85	0.20
	S3	0.55	0.21	0.55	0.12
	S4	0.60	0.23	0.60	0.14

The last column in Table I (relative importance) is formed by the product

$$RI = W \times P \quad . \quad (2)$$

The sum of the relative importance for each task is taken to be the probability for attaining the subgoal S; that is

$$\sum_T RI_T(S) = P(S) \quad . \quad (3)$$

The probability for attaining subgoal IA is 69%.

The effect of eliminating one of the tasks may be seen by making  $P = 0$  for this task. The effect of eliminating S1 is to have a resulting  $P(IA) = 46\%$ , and the effect of eliminating S3 is to have a resulting  $P(IA) = 57\%$ .

The probability for attaining the next goal upward in the pyramid is similarly calculated. A figure of merit is assigned for each subgoal and normalized, so that

$$P(G) = \sum_S RI_S(G) = \sum_S \sum_T W_S(G) RI_T(S) \quad , \quad (4)$$

where  $RI_S(G) = W_S(G) \times P(S)$ , and the total probability becomes

$$P(\text{Total}) = \sum_G W_G (\text{Total}) P(G). \quad (5)$$

The results for chemistry, equation of state, and CJ-Test goals are summarized in Tables II, III, and IV, respectively. Table V summarizes the probabilities for the subgoals, and Table VI summarizes the probabilities for each task in the program, each goal, and the final probabilities.

#### V. CONCLUDING REMARKS

The exercise we have undertaken for the FRE program has been illuminating to us in several ways. First, we were quite surprised at how vividly critical paths expressed themselves in the analysis. Further, the critical paths point out the weaknesses that may exist in the program in terms of lack of manpower, funding, or equipment, perhaps even the recognition that particular areas of technology that are not well developed are essential to the program. Second, we see a strong connection in the generally parallel layout of the FRE program to planning for crisis aversion. This is a characteristic of safety by redundancy that is the hallmark of parallel systems such as the computers on board the space shuttle and back-up systems in general. In the case of the FRE program, the apparent redundancy is far more subtle than having five of the same experiments going on in the false hope that this will improve the chance of success. Many of the tasks in the FRE program feed the same intermediate goals. These tasks are not duplicates of one another but instead provide support and checks to each other. The cumulative result, however, is a degree of redundancy that is healthy in the sense of preventing a failure in one or two tasks from being able to scrub the entire program. Failure of a single task in an inflexible serial system kills the program. Third, it is evident that management can force essentially serial behavior on any program by insufficient funding. Parallelism in a program may appear to be a luxury, but it should also be considered to be insurance toward success. Management may decide on the degree of parallelism to be encouraged in a program by doing



TABLE II  
RELATIVE IMPORTANCE AND SUCCESS PROBABILITIES  
FOR CHEMISTRY TASKS

<u>Subgoal S</u>	<u>Task T</u>	<u>Figure of Merit M</u>	<u>Normalized Figure of Merit W</u>	<u>Probability of Success P</u>	<u>Rel. Importance RI</u>
IA	S1	0.85	0.33	0.70	0.23
	S2	0.60	0.23	0.85	0.20
	S3	0.55	0.21	0.55	0.12
	S4	0.60	0.23	0.60	<u>0.14</u> 0.69
IB	H3	0.90	0.72	0.65	0.47
	T1	0.35	0.28	0.75	<u>0.21</u> 0.68
IC	H2	0.90	0.69	0.75	0.52
	T1	0.40	0.31	0.80	<u>0.25</u> 0.77
ID	T1	0.30	0.20	0.50	0.10
	T2	0.40	0.27	0.55	0.15
	T3	0.80	0.53	0.60	<u>0.32</u> 0.57

TABLE III

RELATIVE IMPORTANCE AND SUCCESS PROBABILITIES  
FOR EQUATION OF STATE TASKS

<u>Subgoal S</u>	<u>Task T</u>	<u>Figure of Merit M</u>	<u>Normalized Figure of Merit W</u>	<u>Probability of Success P</u>	<u>Rel. Importance RI</u>
IIA	H1	0.90	0.36	0.95	0.34
	T1	0.50	0.20	0.90	0.18
	S5	0.55	0.22	0.85	0.19
	T2	0.55	0.22	0.75	<u>0.17</u> 0.88
IIB	H1	0.60	0.17	0.75	0.13
	T1	0.70	0.20	0.80	0.16
	H4	0.85	0.25	0.70	0.18
	S5	0.60	0.17	0.60	0.10
	T2	0.70	0.20	0.75	<u>0.15</u> 0.72
ID	T1	0.60	0.43	0.50	0.22
	T2	0.40	0.28	0.50	0.14
	T3	0.40	0.28	0.50	<u>0.14</u> 0.50

TABLE IV

RELATIVE IMPORTANCE AND SUCCESS PROBABILITIES  
FOR CJ-TEST TASKS

<u>Subgoal S</u>	<u>Task T</u>	<u>Figure of Merit M</u>	<u>Normalized Figure of Merit W</u>	<u>Probability of Success P</u>	<u>Rel. Importance RI</u>
IC	T1	0.00	0.00	0.00	0.00
	H3	0.90	1.00	0.60	<u>0.60</u> 0.60
IIA	H1	0.35	0.47	0.60	0.28
	T1	0.30	0.40	0.50	0.20
	S5	0.00	0.00	0.00	0.00
	T2	0.10	0.13	0.40	<u>0.05</u> 0.53

TABLE V

RELATIVE IMPORTANCE AND SUCCESS PROBABILITIES  
FOR ALL SUBGOALS

Goal G	Subgoal S	Figure of Merit M	Normalized Figure of Merit W	Probability of Sucess P	Rel. Importance RI
Chemistry	IA	0.95	0.46	0.69	0.32
	IB	0.20	0.10	0.68	0.07
	IC	0.30	0.15	0.77	0.12
	ID	0.60	0.29	0.57	<u>0.17</u> 0.68
EOS	IIA	0.80	0.53	0.88	0.47
	IIB	0.20	0.13	0.72	0.09
	ID	0.50	0.33	0.50	<u>0.17</u> 0.73
CJ Test	IC	0.90	0.75	0.60	0.45
	IIA	0.30	0.25	0.53	<u>0.13</u> 0.58

TABLE VI

## SUMMARY OF PROBABILITIES FOR TOTAL PROGRAM

Task	$\underline{P_T}$ (Chemistry)	$\underline{P_T}$ (EOS)	$\underline{P_T}$ (CJ Test)	$\underline{\Sigma W_G P(G)}$
S1	0.11	0.00	0.00	0.07
S2	0.09	0.00	0.00	0.06
S3	0.06	0.00	0.00	0.04
S4	0.06	0.00	0.00	0.04
S5	0.00	0.11	0.00	0.03
T1	0.09	0.19	0.05	0.11
T2	0.04	0.16	0.01	0.07
T3	0.09	0.05	0.00	0.07
H1	0.00	0.20	0.07	0.06
H2	0.08	0.00	0.00	0.05
H3	0.05	0.00	0.45	0.07
H4	<u>0.00</u>	<u>0.02</u>	<u>0.00</u>	<u>0.01</u>
Totals	0.67	0.73	0.58	0.68

M (Chemistry) = 0.80, W (Chemistry) = 0.67

M (EOS) = 0.30, W (EOS) = 0.25

M (CJ Test) = 0.10, W (CJ Test) = 0.08

a cost/benefit analysis that starts with plans of the kind analyzed here for the FRE. It is probable that such an analysis will lead to better estimates of the real costs of successful R&D programs. Fourth, we have found this analysis to be valuable in obtaining a view of an existing R&D program in terms of its current probability of meeting its goals. It is questionable to us whether such an analysis can be accomplished with reasonable accuracy for programs in their proposal stage. In the proposal stage, there is generally insufficiently accurate data or insufficiently well-developed intuition to allow an accurate assessment of probability of success. If an accurate statement of the problem and the approach to solution can be made, it is then possible to decide on initial funding for the program, which is the most important initial management decision. Our analysis yields the important information to motivate and set the level for continued funding of an existing R&D activity but is probably not of much significance in the initial-proposal state except, perhaps, to help define a logical set of tasks and goals. Finally, we note that the final probability of success depends entirely on the accuracy of the input. The estimates of probabilities and weights that constitute the input to the analysis are, in the end, just best guesses. The observation that good researchers are often good guessers is comforting.

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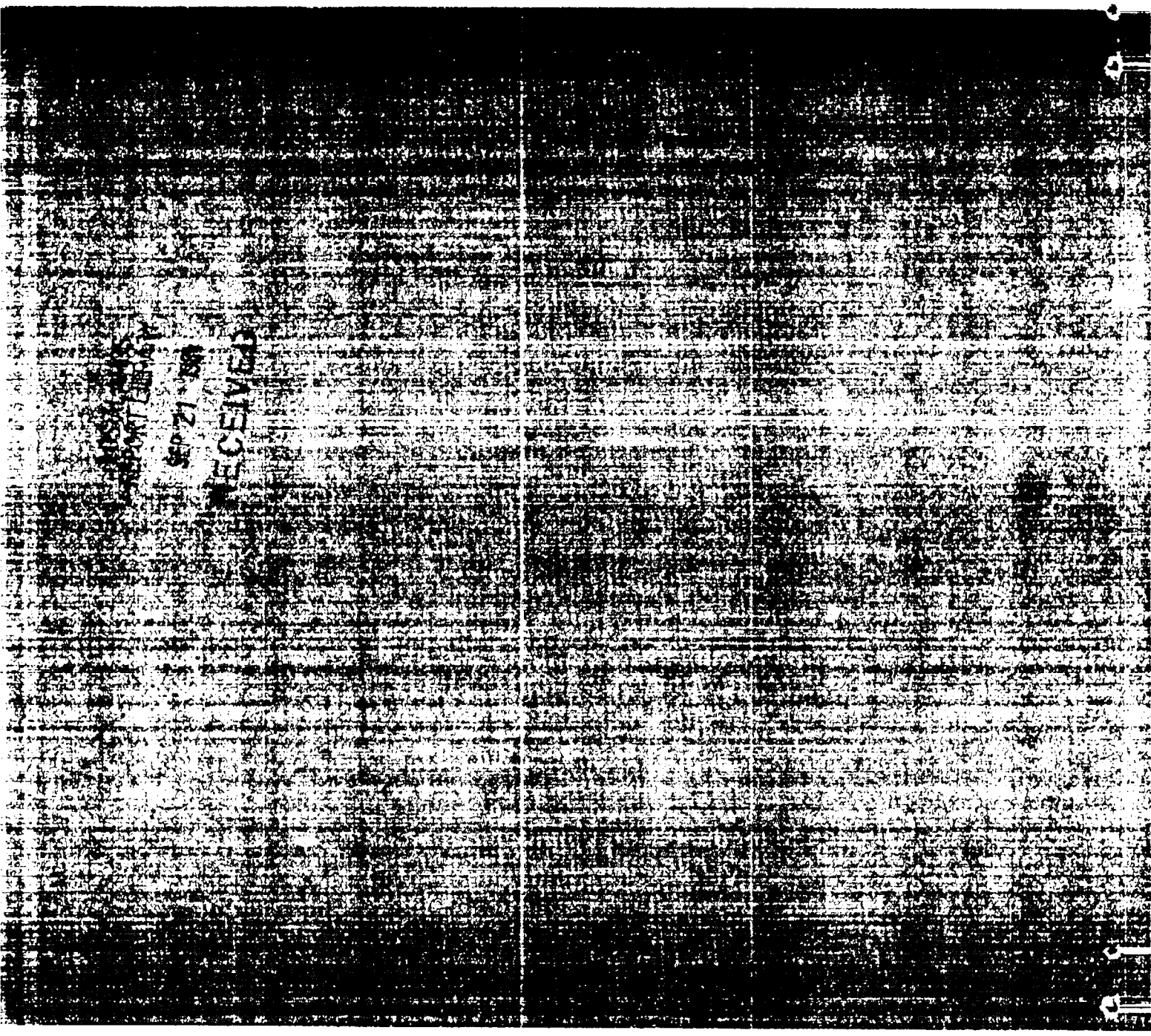
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