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THE USE OF QUALITATIVE AND QUANTITATIVE SIMULATIONS

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ABSTRACT

We describe a technique called *imagining* which uses a combination of qualitative and quantitative simulation techniques to solve a problem where neither alone would suffice. We illustrate the imagining technique using the domain of geologic interpretation and argue for why the two types of simulation are necessary for problems of this sort. We also discuss the strengths of each simulation technique and how they support each other in the problem solving process.

I INTRODUCTION

In solving problems, one often encounters tasks of the sort: "given an initial state, a final state and a possible solution, which is a sequence of events, verify that doing the sequence of events will achieve the goal state". For example, one might want to know whether a proposed sequence of chemical reactions can be used to synthesize a given drug. Essentially, this is the "test" phase of the generate and test method [6]. One common technique for testing the validity of a sequence is to simulate each event in the sequence and to check whether the result of the simulation matches the goal state. This paper investigates using a combination of qualitative and quantitative simulation techniques, which we call *imagining*, in order to test the validity of a sequence of events in domains where neither technique alone would suffice. Imagining is useful for domains in which the goal state is given in quantitative terms but the solution sequence is stated in qualitative terms.

The next section presents our test domain of geologic interpretation and shows how simulation helps solve the problem. Section 3 describes the technique of imagining in more detail. In Section 4, we argue for using a combination of qualitative and quantitative simulations, present the strengths of each and discuss how they support one another.

II GEOLOGIC INTERPRETATION

The domain used as an example throughout this paper is a problem in geology known as *geologic interpretation* [8]. In the geologic interpretation problem, we are given a diagram which represents a cross-section of the Earth (Figure 1a). The task is to infer a sequence of geologic events which plausibly explains how that region came into existence. Figure 1b shows a solution to the cross-section in Figure 1a.

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In [9], we describe a method for generating and testing solutions for the geologic interpretation problem. In this paper, we explore the testing phase in more detail, assuming that solutions of the form shown in Figure 1b have already been generated. The method used to test solutions is to simulate the events in the solution sequence and then to match the final result with the goal state, that is, the diagram cross-section.

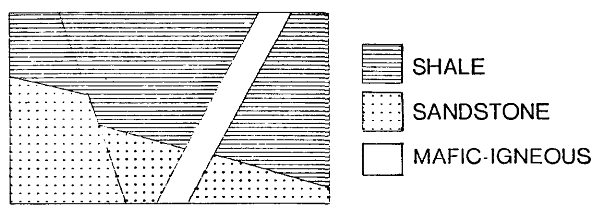
Since our aim is to match the goal diagram with the result of the simulation, it is clearly useful for the simulation to produce a diagram as its result. To accomplish this, a geologic event is simulated by constructing a diagram which represents the spatial effects of that event. For example, simulating the sequence presented in Figure 1b produces the sequence of diagrams in Figure 2. (The initial state, not shown, is a blank diagram, representing the existence of only "bedrock"). Since the final diagram (Figure 2-7) matches the goal diagram (Figure 1a), we can conclude that the solution (Figure 1b) is a valid explanation for how the region came into existence.

III IMAGINING

Imagining is the combined use of qualitative and quantitative simulation techniques to simulate a sequence of events. The diagrams in Figure 2 were produced by doing imagining on the sequence of Figure 1b. In this section, we show how both quantitative and qualitative simulations are used in testing a solution sequence of geologic events.

Fig. 1. Typical Geologic Interpretation Problem and Solution

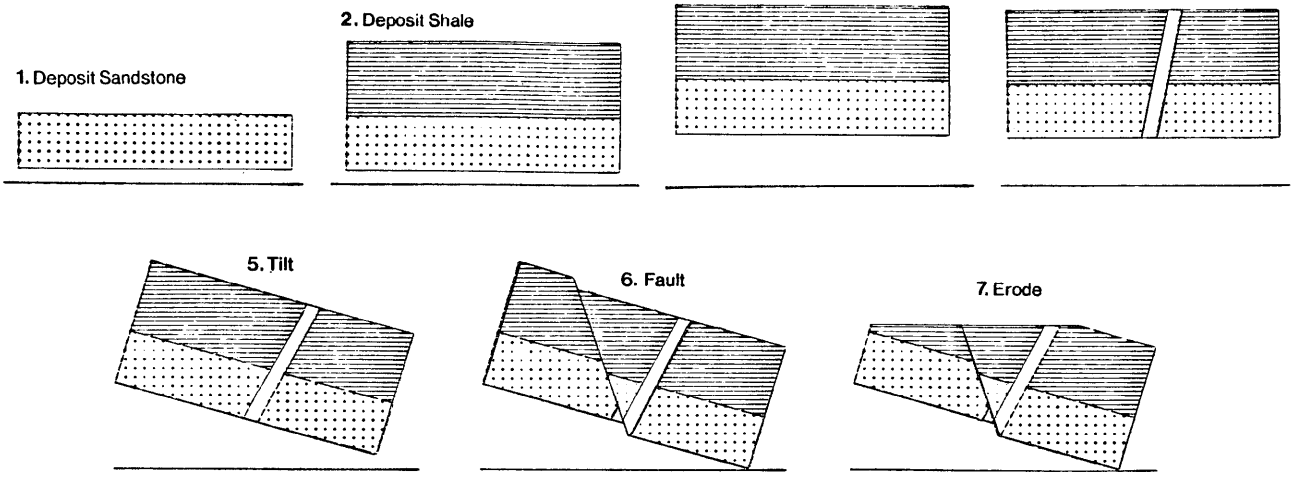
a.



b.

1. Deposit Sandstone
2. Deposit Shale
3. Uplift
4. Intrude Mafic-Igneous
5. Tilt
6. Fault Across Shale and Sandstone
7. Erode Shale and Mafic-Igneous

Fig. 2. Simulation of Sequence in Figure 1b



The technique of constructing a sequence of diagrams is obviously a quantitative simulation technique because diagrams are metric in nature. For example, to simulate deposition we draw a line in the diagram at the level of the top of the deposition (see Figure 2-1). In order to actually draw the line, we must choose an *exact* equation for that line. Since, in our geologic model, the top of deposition is horizontal, the line drawn is completely *parameterized* by the height of the deposition which is being simulated. For each geologic process we have defined process parameters, like the height of deposition, for which numeric values must be chosen in order to construct a diagram that represents the effects of the process. Figure 3 shows the solution of Figure 1b augmented with the numeric parameter values actually used to produce the diagrams of Figure 2.

However, where do the values for these parameters come from? An obvious place to obtain the numeric parameter values is

Fig. 3. Solution to Figure 1a with Parameter Values

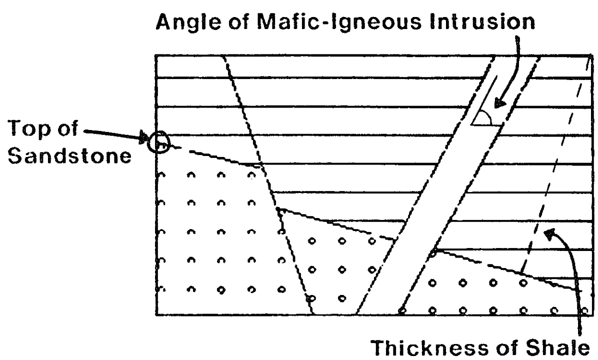
1. Deposit Sandstone to a depth of 450 meters below sea-level.
2. Deposit Shale to a depth of 30 meters below sea-level.
3. Uplift by 200 meters.
4. Intrude 80 meters of Mafic-Igneous at an angle of 78°.
5. Tilt by -16°.
6. Fault at an angle of 108° Across Shale and Sandstone, with a slip of 76 meters.
7. Erode Shale and Mafic-Igneous to sea-level.

to measure them in the goal diagram. For example, the angle of the mafic-igneous intrusion or the thickness of the shale is measurable in the diagram (see Figure 4). But these measurements represent the final values for the parameters -- they might have changed over time due to earlier events. In order to determine the original parameter value we must "correct" for subsequent changes to that parameter, which requires reasoning about the accumulated effects of processes on a parameter.

For example, we need to determine the angle of intrusion of the mafic-igneous (Figure 3, Step 4). Measuring in the goal diagram (Figure 4), we find that the angle is 62°. However, since we know that the intrusion shown in Figure 4 was earlier rotated by -16° due to the tilt (Figure 3, Step 5), we can infer that the actual angle at the time of intrusion was 78°. We use 78° as the parameter value at the time of intrusion so that the later tilt rotates the intrusion to match the angle in the goal diagram. Likewise, the thickness of the shale is measured in the goal diagram as 500 meters, but since we know that some was eroded, the initial amount of deposition must have been greater than 500 meters.

In order to do such reasoning, we need to determine the cumulative changes to the process parameters. This is where the qualitative simulation comes in to play. We can determine the cumulative effects by qualitatively simulating the solution sequence, that is, by symbolically representing the changes that occur to parameters as a result of each event in the sequence. In our case, such changes are represented as symbolic "change equations" which relate, in terms of other parameters, the values of the parameters before and after each event. For example, the changes to the height of the top of the sandstone formation (see

Fig. 4. Measuring from the Diagram



Figures 3 and 4) are given as:

```
height of sandstone top after deposition =
      height of sandstone top before uplift
height of sandstone top after uplift =
      height of sandstone top before uplift
      + uplift-amount
height of sandstone top after uplift =
      height of sandstone top before tilt
height of sandstone top after tilt =
      cos(theta) * height of sandstone
                          top before tilt
     - sin(theta) * lateral of sandstone
                          top before tilt*
height of sandstone top after tilt =
      height of sandstone top in Figure 4
```

Now, to determine the height of the top of the sandstone after deposition, we algebraically manipulate the above equations to obtain:

```
height of sandstone top after deposition =
      [(height of sandstone top in Figure 4
        + sin(theta) * lateral of sandstone
                              top before tilt)
        ÷ cos(theta)]
      - uplift-amount.
```

We now measure the height of the top of the sandstone in Figure 4, and recursively use this technique of measurement and correction to determine the values of the other parameters in the equation (i.e., uplift-amount, lateral of sandstone top and theta, the angle of tilt).

The technique outlined above is the essence of imagining. First, a qualitative simulation is done to establish the cumulative changes to parameters. Second, the results of the simulation (the change equations) and the goal state (the goal diagram) are used to work backwards to infer numeric values for the process parameters. Third, a quantitative simulation is carried out, which in our case constructs a sequence of diagrams, and the final result is matched with the goal state.

IV DISCUSSION

In this section, we argue for the necessity of two kinds of simulation in problems of this sort, discuss the strengths of each and show how they support one another.

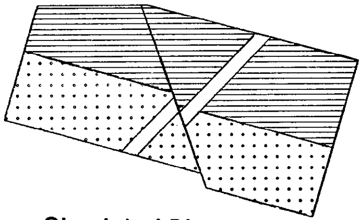
A. Why Two Simulations?

Obviously, doing two simulations is more work than doing one. So why do both? We claim that either alone is inadequate in this domain.

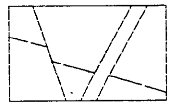
In the previous section we saw that in order to perform the quantitative simulation with parameter values which approximate the values actually used in forming the region, we need to use the symbolic "change equations" obtained from the qualitative simulation to "correct" the values measured in the goal diagram. "Corrected" parameter values are necessary because the process of matching the goal and simulated diagrams is sensitive to the values used. In general, we cannot tell the difference between a mismatch resulting from an incorrect solution sequence and one resulting from the simulation of a valid solution using uncorrected parameter values.

* The "lateral" of a point corresponds to the X coordinate of the point in the diagram.

Fig. 5. Simulation Using Uncorrected Parameter Values



a. Simulated Diagram



b. Goal Diagram

For example, Figure 5a shows a simulation done with parameter values that were measured in the goal diagram (Figure 5b) but not corrected. In comparing Figure 5a with Figure 5b, it is not clear whether the differences arise because the solution sequence is invalid or because the parameter values were badly chosen. Thus, the qualitative simulation is needed to enable us to correct the parameter values used by the quantitative simulation.

Now, let us consider why a qualitative simulation alone will not suffice. One problem is that certain geologic features that help determine a successful match, such as the shape of formations, are difficult to express in qualitative terms. A second problem is that qualitative models are ambiguous, in that a single qualitative representation maps to many real-world situations. For example, if the tilt of a formation is specified qualitatively, such as "tilting clockwise", there is a wide range of actual tilts which match that description. This ambiguity makes the matching problem very difficult. As in other research dealing with qualitative representations (e.g. [2], [3], [4]), we have found that it is necessary to used quantitative knowledge to reduce or eliminate the ambiguities.

The source of both these difficulties is that qualitative representations abstract certain kinds of information, like shape or degree of tilt, and these are precisely the kinds of information needed to determine a successful match. In fact, due to the lack of adequate shape and spatial descriptions, simulating an invalid solution sequence may yield the same *qualitative* result as simulating a valid sequence. Thus, the result of a purely qualitative simulation is totally inadequate for doing the types of matching needed to test solutions for the geologic interpretation problem. We need a quantitative representation of space, which in our case is obtained by constructing diagrams, to perform the matching adequately.

V STRENGTHS OF THE TWO SIMULATION TECHNIQUES

In addition to the fact that each type of simulation is necessary in order to do imagining, both techniques have certain strengths which complement the weaknesses inherent in the other.

For our purposes, the major strength of quantitative simulation is that it produces precise, unambiguous results. It is a fairly simple matter to check for a successful match between the goal diagram and the result of the quantitative simulation. As we have seen in the previous section, the qualitative representation is too abstract to determine a match unambiguously. On the other hand, the abstract nature of the qualitative simulation makes it ideally suited for its task in the imagining technique, which is to enable us to reason about sequences of changes to parameters. Since a qualitative simulation can be performed with much less information than that needed for a quantitative simulation, the qualitative simulation in effect forms a skeleton of the effects of the geologic events and the quantitative simulation allows us to flesh it out.

The major strength of qualitative simulation is that changes are explicitly represented. This facilitates reasoning about what changes occur to parameters. For example, it is much more informative to describe the change to the angle of intrusion of the mafic-igneous as

```
angle of mafic-igneous in Figure 4 =
      angle of mafic-igneous after intrusion
      + angle of tilt
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rather than taking measurements from diagrams and inferring that

$62^{o} = 78^{o} + -16^{o}$.

In fact, composing and manipulating such symbolic equations (see Section III) is precisely what enables us to "correct" the values of the parameters.

A. Process Descriptions

The different uses of the two simulations place strong constraints on how processes are best described. Since it is the end result of the quantitative simulation which is useful, we are concerned primarily that the quantitative process descriptions be computationally simple and robust, that is, they produce accurate simulations over a wide range of inputs. The qualitative simulation is used primarily to accumulate the changes to parameters, and so the process descriptions should explicitly represent the effects of the processes. These constraints have led us to develop quantitative process descriptions which are algorithmic or "do this" descriptions, whereas qualitative process descriptions are assertional or "what happens" descriptions. Figure 6 illustrates the flavor of our quantitative and qualitative descriptions of deposition.* Notice how concisely we can describe deposition algorithmically. In general, it is much easier to come up with an algorithmic description of a process than to find an assertional description. This is one reason why quantitative simulation techniques have been used for a long time (e.g SIMULA [1]). Also, there are usually efficient methods for "running" these algorithms on quantitative representations, thus effecting the simulation.

Recently much work has been done on qualitative representations and simulation (e.g. [2], [3], [4], [5], [7]; this work owes much to these pioneering efforts). That research, as well as our own, has pointed out the difficulty of formulating a qualitative description of a process which completely captures the effects of the process. For example, we have been unable to come up with an adequate qualitative description of shape and,

* See [10] for a more complete description.

Fig. 6. Quantitative and Qualitative Descriptions of Deposition

A. QUANTITATIVE ALGORITHM FOR DOING DEPOSITION

1. Find the lowest end-point of all the edges that represent the surface of the Earth.
2. Draw a horizontal line "DLEVEL" above that.
3. Erase all parts of the line that cut across a face corresponding to a rock-unit.
4. All other newly created faces below the line are part of the newly created sedimentary rock-unit.

B. QUALITATIVE PROCESS DESCRIPTION OF THE CHANGES DUE TO DEPOSITION

1. The thickness of the deposit is "DLEVEL minus the height of the bottom of the Earth's surface at the start of deposition".
2. The orientation of the deposit is zero.
3. There is a boundary between the deposit and all formations which are on the Earth's surface at the start of deposition and whose bottoms are below DLEVEL.
4. The composition of the deposit is DCOMPOSITION.
5. The bottom of the deposit is the same as the bottom of the Earth's surface at the start of deposition.
6. The top of the deposit is the same as the bottom of the Earth's surface at the end of deposition.
7. The height of the bottom of the Earth's surface at the end of deposition is DLEVEL.
8. The height of the top of the deposit at the end of deposition is less than sea-level.

in fact, in Figure 6b there are no assertions concerning how the shape of the deposited formation changes. Fortunately, shape is easily represented using diagrams and so all shape changes are inferred by referring to the diagram. On the other hand, the assertional nature of the qualitative process description makes it very easy to change a description. We can independently add or modify individual assertions as our understanding of the process increases. This has proven to be very useful in our research.

B. Associations Between the Two Simulations

Qualitative descriptions are difficult to develop because we need a good understanding of what happens to the world when the process occurs. It turns out that doing the *quantitative* simulation is very useful in developing qualitative process descriptions. Since the accumulated changes produced by the qualitative simulation are used to correct the parameter values, a missing change will yield an incorrect value, causing a quantitative difference between the simulated and the goal diagrams. Thus, we can "see" the effects of incomplete qualitative process descriptions.

For example, Figure 7a was produced using a process description of faulting which did not include the fact that the rocks on one side of the fault slide downward. Although the simulated diagram topologically resembles the goal diagram (Figure 7b), when we superimpose the two (Figure 7c) we see that the incomplete description of faulting causes a slight quantitative inaccuracy in the simulated diagram. In particular, the mafic-igneous intrusion is lower than in the goal diagram (Figure 7b) because its displacement due to the fault sliding was not accounted for when correcting the parameter value for the height of the mafic-igneous.

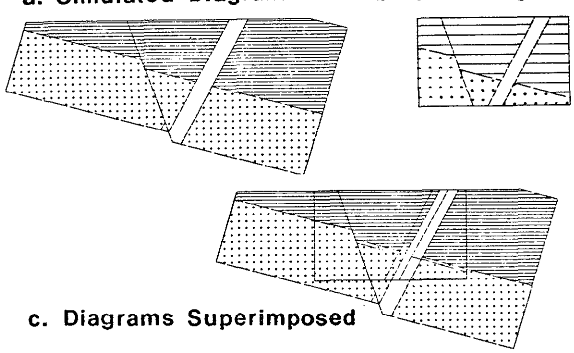
Although it is not trivial to determine the source of the error from the difference between the two diagrams, the comparison does provide an indication of which parameter is inaccurate. By checking the sequence of changes for that parameter against our own geologic knowledge of what was supposed to happen, we can usually pinpoint which process description is incomplete and in what ways. For example, we can determine that the process description of faulting is the one which is incomplete by noting that the diagram associated with the faulting is the first one in the sequence of simulated diagrams in which the actual height of the mafic-igneous differs from the height predicted by the imaginer. This pinpoints that the faulting process is incomplete and that the error has something to do with changing the height of existing rocks. From our knowledge of geology we would realize that the missing change is that the rocks on one side of the fault slide downwards. By applying this methodology over several geologic interpretation examples, our models and understanding of the geologic processes have become greatly refined.

Notice that in *using* the system to test the validity of sequences, the qualitative simulation is needed in order to perform the quantitative simulation accurately. However, in *developing* the system, the quantitative simulation supports the qualitative by enabling us to "see" the bugs in our qualitative process descriptions.

C. Multiple Representations and Other Issues

Many of the ideas expressed in this paper are treated in more detail in [10]. In that paper, particular attention is paid to the multiple representations needed to support the qualitative and quantitative simulations, how these representations are used and how they interact. One interesting result discussed there concerns process parameters which are not measurable in the diagram, such as the amount of uplift or the amount of erosion. It is shown that for those parameters any arbitrary value may be chosen without affecting the final diagram produced by the quantitative simulation.

Fig. 7. Simulation Using Incomplete Process Description



a. Simulated Diagram **b. Goal Diagram**

c. Diagrams Superimposed

We believe that imagining could prove useful in other domains as well. For example, an economist might test a theory of how the economy reached its current (quantitative) state by seeing if the results predicted by the theory match the current economic state. Other domains involve scientific experimentation in areas such as biology or chemistry, where experiments are run, data are collected and a sequence of events is proposed to explain the data. The scientist might then use imagining to test whether the proposed sequence would result in the same test data.

VI CONCLUSIONS

We have developed a new technique, called *imagining*, which uses a combination of qualitative and quantitative simulations to solve problems in domains where neither technique alone is adequate. The basic technique of imagining involves three steps. First, a qualitative simulation is performed to establish the sequence of changes to process parameters. Second, the result of the simulation, represented as "change equations", and the goal state are used to work backwards to infer numeric values for the process parameters. Third, a quantitative simulation is carried out and the final result is matched with the goal state. We believe that imagining will prove useful in testing the validity of a sequence of events in domains where the goal state is given in quantitative terms and the sequence of events is given in qualitative terms.

VII ACKNOWLEDGEMENTS

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