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Presented at the 1986 Fall Meeting of the
American Geophysical Union, Symposium on Flow and
Transport through Unsaturated Fractured Rock,
San Francisco, CA, December 8–12, 1986

SOME THOUGHTS ON MODEL VERIFICATION

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February 1987

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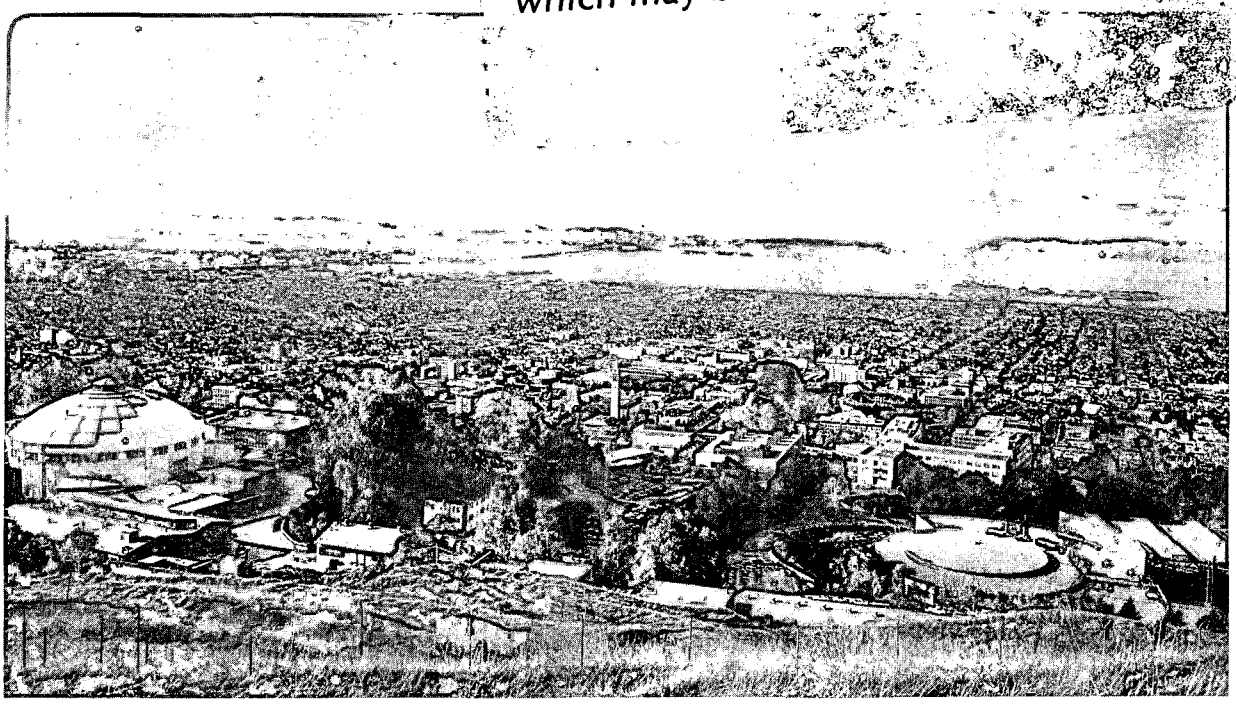

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Prepared for the U.S. Department of Energy under Contract DE-AC03-76SF00098

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LBL-23021

Some Thoughts On Model Verification

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This work was supported by the
U.S. Department of Energy under Contract No. DE-AC03-76SF0098

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ABSTRACT

The most powerful attribute of numerical models for simulating fluid flow in partially saturated fractured media is that they can handle arbitrarily complex problems in terms of geometry, heterogeneity and forcing functions. In contrast, analytical solutions can be only obtained for relatively simple problems. Therefore, the very power of the numerical models that is to be exploited is unnecessarily abridged if the numerical method is viewed merely as a tool for approximately solving the partial differential equation. A broader definition of verification is needed in order to exploit the power and generality of numerical models. In the ultimate, verification should be dictated by axiomatic testability. The development of self-verifying numerical models is a challenge that deserves pursuit.

INTRODUCTION

This essay summarizes certain perspectives expressed by the author during a panel discussion. The discussion occurred at the end of the Special Session entitled," Flow and Transport through Unsaturated Fractured Rocks" held during the Fall Meeting of the American Geophysical Union, San Francisco, December 8-12, 1986. A majority of the papers presented during the session related to the flow of water in partially saturated fractured porous media. The panel discussion which helped wrap up the session was aimed at identifying key issues of interest and to provoke discussion among the participants.

In the context of the panel discussion, the author's charge was to address mathematical modeling. This topic being very broad in scope, it was decided to focus discussion on one important aspect of modeling, namely, *verification*. As used here, the term, *verification*, refers to that task by which a mathematical solution to an arbitrarily complex problem is tested for internal mathematical consistency and accuracy. This notion is distinct from the related one of validation, which relates to the closeness of

similarity between the mathematical model and the physical system which it seeks to represent. In the present essay we will first present the context in which mathematical models are used to study flow and transport in unsaturated fractured rocks. We will then discuss the issue of *verification*.

THE CONTEXT

In the present context, models can be viewed from two broad view points: the physical content of models on the one hand and the mathematical representation of the physical content on the other. In so far as the the physical content is concerned we are dealing with systems charaterised by heterogeneities, especially introduced by the presence of fractures, in a host rock that may be porous. Superposed on the heterogeneous system are the effects of flow characterized by the presence of more than one fluid phase. The motion of fluids in multiphase systems is dominated by the complex surface interactions and energy transfers that occur between the fluid phases themselves and between the fluids and the solid phases. Perhaps the simplest multiphase system that is of interest to us is the air-water system in which the air phase is assumed to be everywhere at atmospheric pressure. Such a system has been traditionally represented by what is known as Richards Equation in the soil science literature (Richards, 1931)

Starting from the late 1960's many attempts have been made to implement and solve Richards equation through mathematical models. Invoking such techniques as Finite Differences, Finite Elements, Integral Finite Differences and the Boundary Elements , the numerical models have since been applied to a wide variety of problems in many earth science disciplines. Within the last decade an effort has been made by some workers to extend Richards equation to systems which contain fractures. A key conceptual element in this extension is the recognition that natural fractures are characterized by rough walls and that the walls may have discrete points of contact, usually known as asperities. As a consequence of the roughness, the fracture opening or aperture is a spatially variable function. In a fractured porous medium such as a fractured shale, fractured sandstone or fractured tuff, the fracture apertures are in general likely to be larger than the pore openings.

A fractured porous medium can therefore be viewed as a heterogeneous system with bimodal pore population: the fractures constitute one population with relatively large openings and the host rock consitutes another with relatively small openings. As soon as we idealize the fractured porous medium in this way, we can apply to this system the capillary theory on which Richards equation is founded. This conceptualization is now being used by some (e.g. Wang and Narasimhan, 1985) to model fluid flow in unsaturated fractured rocks.

A related notion that is relevant in fractured porous media is that when fractured porous media are fully saturated with water, the migration of water will be very rapid in the fractures and be significantly slower in the matrix. One way of quantifying this difference in the behavior of the fractures and the matrix is to state that the fractures have very small time constants relative to the matrix. The *time constant or, the reaction time,* can be defined as the ratio of the capacitance of a subdomain to its conductance. The fractures, characterized by large hydraulic conductivities and very low storativities will have very small time constants as compared to the rock matrix characterized by vastly larger storativities and much smaller conductivities. The physical response of these systems to transport processes can be unique and may not admit of representation by an equivalent homogeneous system. Following a lead provided by Barenblatt et al (1960), Pruess and Narasimhan (1985) suggested a modeling technique by which systems with heterogeneities with widely differing time constants could be conveniently handled. Termed MINC for *Multiple Interacting Continua,* this modeling approach chooses to treat the interconnected fractures as one continuum and to treat the rock matrix as several nested continua, as dictated by the proximity to fracture surface. The transient interaction between these several continua is determined not only by the transport properties of the continua but also by the *geometry* of the continua.

The implementation of Richards equation or the MINC concept can be achieved by using any of the existing techniques such as finite differences, integral finite differences or finite elements. As a setting for discussing the issue of verification, we will assume that we now have a variety of computer algorithms to model flow and transport in unsaturated fractured rocks. Here, we concern ourselves with those issues that constitute a

common denominator to all these models. In particular, we will address the issues that relate to the modeling aspects rather than the physical content of the governing equations itself.

VERIFICATION

Central to the issue of verification are the questions,

Is the algorithm accurately solving the mathematical problem? How can one assert that it does?

In order to address these questions, we need to start by considering the philosophy that underlies the construction of mathematical models as we now use them. As a consequence of the continuum concepts that were introduced into classical science more than a century or two ago, we start with the underlying premise that physical systems such the one represented by Richards equation are represented by a set of partial differential equations. If so, one may naturally treat numerical models as tools that help to approximately solve the appropriate set of partial differential equations. A corollary of this perspective is that if one wishes to *verify* or, equivalently, *assert* that the solution is correct, then one has to show that the numerical solution very closely approximates the analytical solution to the differential equation. We tacitly assume that analytic solutions *can be* obtained to the problem of interest and that such solutions can *readily asserted* to be the correct solutions. Almost all current modeling effort related to fluid flow and transport are founded on this tenet.

The disconcerting aspect of this foundation is that for almost all realistic problems that deal with unsaturated flow and transport in fractured porous media, no mathematical techniques have been developed for obtaining analytical solutions. The realistic problems are characterized by complex geometries, very strong nonlinearities and strong time-dependence. As a result, there is no established way of verifying numerical solutions at the present time when the nature of the particular problem is more complex than that of related analytic solutions.

As a consequence, the current status of modeling with reference to verification is twofold. In the first, the commonly followed approach, one simply tests the model against the most complicated analytical solution that one has access to and then assumes that the model solution for any other new problem should be correct or credible. The second approach, not often followed, is to solve the problem numerically with as many grid points as possible. The logic being, *the finer the discretization, the better the agreement with the analytic solution.*

In applied earth sciences, models such as those that are addressed in this essay are used in either of two ways. One may use models to gain qualitative insights into problems that are so complicated that they are beyond the scope of the largest available computers or the most comprehensive data bases extant. Or, one may use models to make quantitative and semiquantitative predictions to aid in engineering decisions. The issue of verification assumes special significance in the latter case. Models are receiving enormous attention as potentially capable of helping to solve complex problems that are of national interest. A good example involving flow and transport in unsaturated fractured rocks is that of toxic or radioactive waste disposal. Enormous resources are being spent on calculations using models. Yet there is no fundamentally sound procedure for verifying model solutions. Thus, this status is disturbing, not purely for scientific reasons. When model results are used to make decisions that are socially sensitive, the credibility of model results is of extraordinary importance. It is of considerable scientific and practical interest to ask whether special attention should be paid to enhance our ability to verify our models. The current approach towards this enhancement is simply to enlarge our repertoir of available analytical solutions.

A strong motivation for presenting this essay is to suggest that we should reexamine our fundamental philosophy of modeling in order to enhance our ability to verify. Development and use of methodologies that defy verification go against the grain of modern scientific thought. For, the essence of modern science is that any scientific statement must be testable against fundmanetal postulates. Therefore, it is of fundmaental interest to ask the question,

Is it possible to devise numerical models that are self-verifying ?

A SUGGESTION

If we examine our current foundations of numerical modeling, we find that many of our numerical difficulties such as spatial truncation errors and time-truncation errors directly stem from the need to evaluate gradients, especially in space, of potential fields. This, in turn, is a consequence of the fact that we have chosen to express the physical phenomena in terms of gradients and the differential equation. Yet the basic laws of nature, in our case those represented by the laws of Newtonian mechanics, do not necessarily *demand* the use of derivatives and differential equations for their expression. Indeed, it is possible that by drawing upon a priori knowledge of the kinematics and the geometry of the system one can express the governing statement of the physical systems in such a way that the use of gradients and derivatives are either excluded or greatly reduced. Will such direct integral representations of the physical system and the numerical evaluation of these integrals as disctrete sums provide opportunities for developing *self-verifying* mathematical models?

The answer seems to be in the affirmative. Recent work by the author (Narasimhan, 1985) at least suggest the possibility that computational reliability and efficiency can be enhanced by merely using the known geometric aspects of the system. There is even a suggestion that the essence of solving the transient fluid flow process is that of solving for the *geometry of the flow system,* rather than the traditional notion of solving for the potential. At the level of formulating the governing equations it will be more profitable to invest effort to increase the information content of the integral equation, than to use the integral as a dispensable intermediate step towards deriving the differential equation.

Upon reflection it is not unreasonable to state that our enterprise of numerical modeling is at present treated as a means of approximation to one branch of mathematics, namely functional analysis. This branch is certainly most compatible with the task of obtaining solutions by analytic methods. Nevertheless, it is likely that for direct

evaluation integral statements and their verification, it may be more advantageous to seek other branches of mathematics such as measure and integration.

In the case of analytic solutions, when available, the notion of verification merely consists in checking whether the spatial derivatives of the function called a solution exactly matches its temporal derivative. No such simple verification logic is available for numerical solutions. The best way to overcome this difficulty is to take a broader view of the notion of verification and to associate it with the task of assuring that the computational operations of discrete integrals are consistent with the governing axioms of change of state, motion and conservation.

CONCLUDING REMARK

In its essence modern science is based on axiomatic logic. Any scientific theory or statement must permit of being tested against a set of governing axioms. Our enterprise of numerical modeling should take to this logic as a sound basis for verification rather than taking the much narrower view in which conformity with an analytical solution is considered the basis for verification. It is suggested that in the modern world of super-fast computing, significant advantages may be gained by devoting more attention to using integral equations in their own right, rather than treating them as extensions of differential equations. Much could be gained by attempting to develop logical systems that can exist totally independently of the differential equation

ACKNOWLEDGEMENTS

Thanks are due to Mark McGuinness, K. Pruess, C.F. Tsang, and J.S.Y. Wang for reviewing the manuscript. This work was supported through U.S. Department of Energy Contract No. DE-AC03-76SF00098 by the Assistant Secretary for Energy Research, Office of Basic Energy Sciences, Division of Engineering and Geosciences.

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This report was done with support from the Department of Energy. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the Department of Energy.

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