COMPUTATIONAL BIOPSY TO ASSESS ACCURACY OF LARGE SCALE COMPUTATIONAL GROUNDWATER FLOW MODELS

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ABSTRACT

Due to the availability of comprehensive computational models of various computer modeling approaches to solving problems in computational engineering, mathematics, and science, and also due to the capacity of modern computers to computational solve the governing mathematical relationships involved in the problem solving procedures, the use of methods in Computational Engineering Mathematics to solve such problems has become a new standard of care in the design process as well as planning. However, sometimes the computational results are not sufficiently accurate or may be solving an alternate problem than what was contemplated. In this work, we propose the concept of "computational biopsy" where small portions of the global model are identified where a test problem is inserted into the global model and then the global model is rerun with the inserted test problems in place, producing another set of computational results that include the small inserted test problems. For properly selected test problems, exact solutions typically exist and can be compared to the computational results obtained from the global model as modified to contain the inserted test problems.

Keywords: *Computational domain, FROST2D, SEEP/W, transient profiles*

1. INTRODUCTION

The use of computational models for the analysis of complex problems in small and large scale problems continues to gain in common usage in modern engineering design and planning. Background into the procedures and computational approaches used in such computational modeling approaches are thoroughly reviewed, and computer code provided in FORTRAN, in the book by C.A. Brebbia and A.J. Ferrante [1] entitled "Computational Hydraulics". Other texts and publications are available in the literature, but the book by Brebbia provides a particularly detailed and practical assessment of the technology still in modern use. As a result of such widespread use of computational models to solve problems in fluid transport processes, including but by no means limited to groundwater saturated and unsaturated flow in soils, experience with such computational approaches has accumulated. Additionally, commonly occurring difficulties (such as inadequate computational accuracy in predicting rapidly changing variables, among other issues) in the use and application of such computational models has drawn attention towards research in methods to reduce the impacts and occurrence of such modeling issues.

In the J. Hydraulic Research, Vol. 14, the research article entitled, "Computational Hydraulics: A Short Pathology" [2], states that "Several members of the IAHR section on the use of computers in hydraulics and water resources have expressed concern at the quality of many of the computational models currently used in hydraulic research and hydraulic and coastal engineering practice. The purpose of this article is to explain some of the grounds for their concern by illustrating some of the errors that commonly occur in this type of work...Difficulties and errors arise not only in the models themselves but also in their applications. Unless the entire investigation operation functions correctly, the consequences of these errors can be very serious in engineering practice. Finally, the need for more education in this area is emphasized." This paper was followed by the research article, "Computational Hydraulics: An Alternative View" published by M.B. Abbott et al in J. Hydraulic Research in Jan, 2010, which further examines issues involving modeling complexity and large scale modeling issues. In the second paper, a distinction is made between "traditional" modeling approaches that assess the entire global problem domain, versus a more modeling focused approach, or "alternative" methods, that concentrate modeling effort at the smaller but more involved hydraulic and transport process locations. Abbott et al [3] write that, "...The traditional approach can be used most efficiently when, roughly speaking, the same order of variation occurs in the dependent variables over most of the domain during most of the time. In a large number of real-life situations, however, nothing much happens in most of the domain during most of the time but the areas of interest are concentrated in small regions that may move across the domain in time. Examples are the spillage, transport and dispersion of pollutants in watercourses, the propagation of Tsunamis waves, halocline and thermocline decay, bio-chemical process at air-water and bed-water interfaces and haloclines and also the transport of short wave energy. The alternative methods provide a generally superior resolution in these situations, as compared with the traditional ones, but this advantage is bought at the cost of an increased complexity of the numerical scheme or code. Applications are shown to the transport processes, dispersion process and conservation (propagation) processes of hydraulics, so covering most common applications...".

In the current paper, an approach for assessing computational models of fluid transport, such as commonly encountered in the analysis of saturated and unsaturated groundwater (or soil-water) flow in soils, with or without soil-water phase change due to freezing and thawing effects, is considered by testing the global computational model through introduction and insertion of several test situations within the global problem domain where analytic solutions to the test problem is available. The revised global model is then re-run to obtain an alternative solution outcome that can then be assessed as to the revised global model's computational accuracy in predicting the computational results corresponding to the individual test problems. The focus of this assessment is at the test problem locations. Such specific location tests can be applied throughout the global model where, as distinguished by Abbot, "... the areas of interest are concentrated in small regions that may move across the domain in time..." These tests are referred to in this paper as computational "biopsies" in that small and specifically selected locations within the global computational model are being examined individually rather than the entire global model. Different tests can be conducted at these biopsy locations by modification of the boundary and initial conditions of the transport equation test problem selected. And similar to the usual biological biopsy procedure, the success in the alternative or modified global model in achieving good computational results for the selected test problem is a "necessary" condition for global model success, but is not a "sufficient" condition to assure overall global model success.

Examples of computational model difficulties are presented in the Lecture entitled "Introduction to Computational Mathematics" [4]. In that lecture, standard computational issues are examined as well as complex topics. Of course, such computational issues continue to survive even today in the most modern computational models that are commonly used in design and planning of engineering and other works. In other words, the computational modeler still must address the same issues and difficulties (such as computational issues regarding stability, convergence, and consistency) in using computational models such as existed in the past, even though the computational modeling outcome is incredibly detailed because of modern visualization techniques.

Phil Roe, Professor of Aerospace Engineering at the University of Michigan published his video lecture on Feb. 19, 2014 entitled, "Colorful Fluid Dynamics", dealing with topics of modern Computational Fluid Dynamics ("CFD"), and mentions, "It's full of noise, it's full of color, it's spectacular, it's intended to blow your mind away, it's intended to disarm criticism." Roe then discusses some issues with CFD and the dangers of "colorful fluid dynamics", and references the statement by Doug McLean (for example, video lecture "Common Misconceptions in Aerodynamics", Oct 21, 2013, among other publications, retired Boeing Technical Fellow): "These days it is common to see a complicated flow field, predicted with all the right general features and displayed in glorious detail that looks like the real thing. Results viewed in this way take on an air of authority out of proportion to their accuracy...". The Computational Biopsy approach aids to illuminate possible sources of computational modeling error by demonstrating the magnitude of such errors using a well-known and well-understood test problem or set of problems.

Given the experiences with such computational modeling, there is value in developing methods to assess the potential of such computational issues occurring within an application of a computational model, such as modeling transport processes such as soil-water flow in saturated and unsaturated soils. Additionally, education is needed to highlight such computational issues in order to alert computational modelers that experience and advanced knowledge of the underpinnings involved in a selected computational model is still needed, even though the computational modeling outcome appears to be plausible and seem strikingly realistic. That is, there is still considerable need to know many of the elements of mathematics and computational methods that are studied in courses found in university programs of computational engineering mathematics.

2. CASE STUDY: ASSESSMENT OF GROUNDWATER FLOW USING TWO COMPUTATIONAL MODELS

For the current work, two computational models of groundwater flow are examined. The models selected to demonstrate the computational biopsy approach are computer program FROST2D and also computer program SEEP/W. Both computer codes solve the usual saturated and unsaturated flow equations of soil water movement in soils. Program FROST2D solves the coupled saturated and unsaturated soil water flow equations in a two-dimensional problem domain. The program includes an algorithm for modeling soil water phase change, however that process is not assessed in the current work. The computer code in FROST2D software (Guymon et al. 1993) was developed as part of a research effort funded in the later 1970's and early 1980's by the U S army Corps of Engineers Cold Regions Research and Engineering Laboratory (CRREL) and has been in use since its inception for a variety of problems. Program SEEP/W (Krahn 2012) is a world-wide distributed computer code for solving saturated and also unsaturated soil water flow in two-dimensional soil problem domains. Because both computer codes have been in use by a variety of end-users and because the FROST2D program has a long history of availability, the assessment of both programs in their application to a common problem may provide an interesting comparison in computational efficiency as well as accuracy. Both programs are applied to the same two-dimensional problem, and then both global models are then examined using the same "computational biopsy" test locations within the respective models. The resulting assessment is a comparison between three computational model sets of results in solving the identical test problem, including computational results from the two computer codes selected for examination, and computational results from the biopsy test problem which in this particular case has an exact solution available. The computational results from the selected test problem serve as a "baseline" to use in assessing modeling performance. More details regarding the biopsy test problem are provided in a following section.

The two-dimensional groundwater flow equation for coupled saturated and unsaturated soil water flow is given by Eq. (1),

$$C\frac{\partial \emptyset}{\partial t} = \frac{\partial}{\partial x}\left(K_x \frac{\partial \emptyset}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial \emptyset}{\partial y}\right) \quad (1)$$

Where, C is a capacitance coefficient; x, y, and z are the spatial coordinates; t is the model time coordinate; $\emptyset$ is the potential function; K_i for i = x, y is the hydraulic conductivity, with each subscript denoting the specific coordinate direction.

The three-dimensional formulation is readily obtained by simply including the third dimension flow transport term. Sources and sinks are not included in Eq. (1). Both computational programs FROST2D and SEEP/W numerically solve Eq. (1) given initial and boundary conditions appropriately defined.

3. THE SELECTED "COMPUTATIONAL BIOPSY" TEST AND RESULTS

The selected test situation is a one-dimensional diffusion transport model, such as used to describe one-dimension heat transport in a long rod. To apply this test scenario, locations are selected within the global model problem domain where the test problem can be included into the global model and where also the modified global model is not significantly altered except at the location of the "biopsy". In this way, the modified global model can be re-run as originally envisaged, but with the inserted test problems being solved as part of the global modeling solution effort. That is, the original global modeling computational discretization scheme and numerical algorithms employed remain in use as originally set up, but now the inserted test problems are being concurrently analyzed by the same computational global model.

The test problem (or test situation) being used for this work is the classic one-dimensional transient heat transfer problem with initial conditions at normalized model time t=0 defined as value 1.0, and with boundary conditions defined at normalized locations x = 0 and x = 1 with value 0. The governing partial differential equation describing the heat transfer problem is given in Eq. (2). The analytic solution of the test problem is the series given in Eq. (3).

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{\partial u}{\partial t} \quad (2)$$

$$u(x,t) = \frac{4u_o}{\pi}\sum_{n=1}^{3}\frac{\sin\left((2n-1)\pi x\right)}{(2n-1)}\exp(-(2n-1)^2\pi^2 t) \quad (3)$$

The similarity between the groundwater flow Eq. (1) and the selected test heat transport Eq. (2) is apparent. Other test problems can be used instead of the test problem selected for the current effort, where a suite of test problems can be formulated by revising initial conditions and boundary conditions, for example.

Figures 1 and 2 display the test problem computational results that are available with the analytic solution described by the generalized Fourier series shown in Eq. (3). In these Figures, the analytic solution as well as computational solutions developed by EXCEL, are compared. The figures compare computational results between the target computer programs FROST2D, SEEP/W, the analytic solution, and an (Microsoft) EXCEL computational model of the analytic solution. Convergence is examined by use and comparison of a 10 -node and also a 203-node computational discretization for all the models considered. As seen in the Figures 1 and 2, a higher level of discretization results in significantly improved computational results for the test problem examined. Furthermore, the computer programs SEEP/W and FROST2D both show significant improvement in their computational results for the increased level of discretization. Although it is true that these computational results in assessing convergence of the modeling can be obtained by simply increasing the level of discretization, it is also true that for large scale applications of such models involving perhaps millions of computational elements, that increasing the level of discretization may be prohibitive. In such cases, among others, the considered computational biopsy approach for examining the veracity of computational results may be a useful approach for examining modeling accuracy.

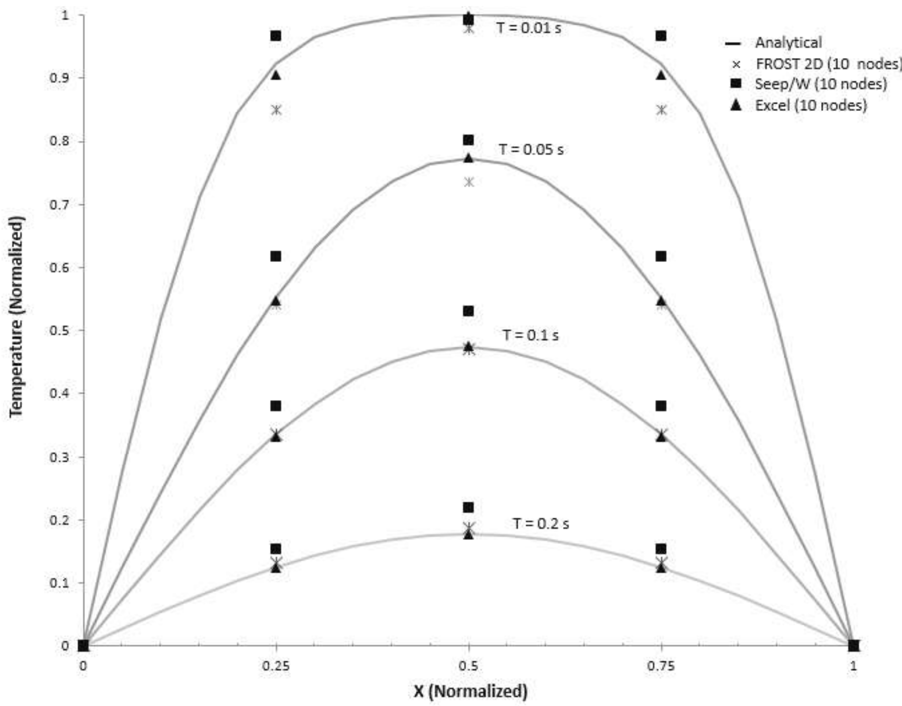

Figure 1. Comparison of Analytical, Frost2D, Seep/W and Excel solution (Number of nodes = 10)

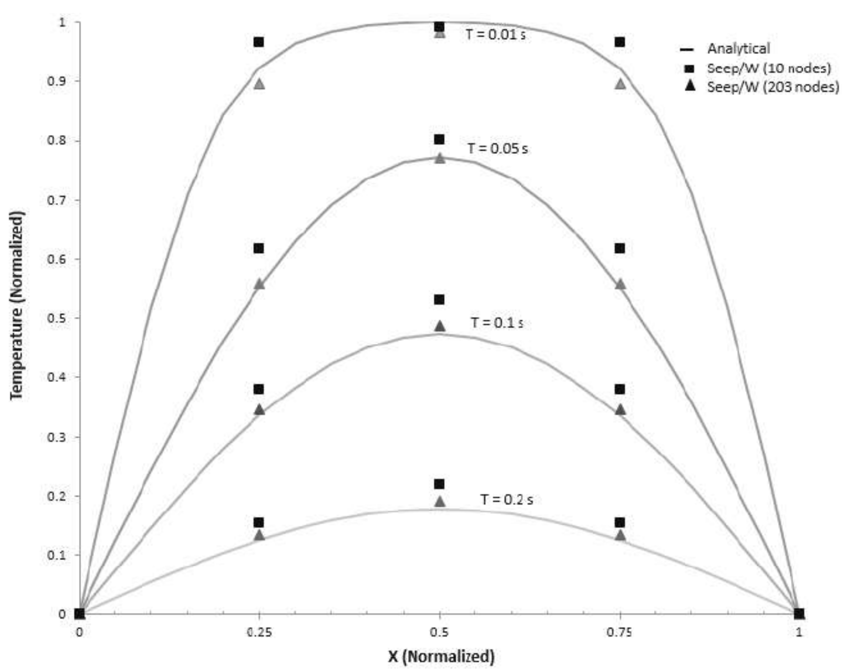

Figure 2. Sensitivity of Seep/w solution for 10 and 203 nodes in the computational domain

These various computational and analytic results can be used directly to compare with the two selected global computer models. Once the test problem is properly inserted into the global computational model, additional tests can be readily obtained by changing the test problem boundary conditions and initial conditions. Of course, such changes would necessitate re-running the global model in order to properly include the new test situations. Other computational biopsy locations can be examined by simply inserting the selected test problem situation into the global model and re-running.

4. CONCLUSION

A reproducible approach towards assessing computational veracity of large scale computational models is presented for the case of groundwater or soil-water flow modeling. The approach is called "computational biopsy" where samples of the global computational model are examined as to computational veracity using test situations where analytic solutions exists. Although use of several test locations and test situations may increase confidence in the global modeling computational results and their accuracy, such tests only provide a "necessary" condition is assessing modeling veracity and not a "sufficient" condition for the purposes of describing overall global modeling success.

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