ON THE RELIABILITY AND ACCURACY OF COMPUTATIONAL MODELS FOR HYDROSCIENCE AND ENGINEERING INVESTIGATIONS

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ABSTRACT

More computational models have been developed for applications to the investigations of a variety of problems in hydroscience and engineering. Some of them have been utilized in not only engineering designs; but also planning, management and even policy decisions of large scale and highly complex projects costing huge amounts of funds and having long-term impact to our society. The lack of a rigorous methodology for establishing the quality standard, or the assurance of the models' reliability and accuracy, has raised great concerns by a number of professional societies, research institutions, governmental agencies and professionals in the field worldwide.

This paper is to introduce the findings of the ASCE-EWRI Task Committee on 3D Free Surface Flow Model Verification and Validation. The Task Committee consisting of more than 15 members from 6 countries have actively worked on this task for more than 8 years. The detailed findings shall be soon published in an ASCE Monograph on this topic. The paper intends to present only the highlights briefly.

A rigorous validation and verification process of computational model for hydro-engineering investigations should include three steps: Mathematical Verification, Physical Process Validation, and Site/Case-Specific Validation. The Mathematical Verification Step is primarily to assure that the model being tested does not have mathematical derivation and solution mistakes and coding errors. It can also determine the accuracy of simulation results and errors of computation quantitatively. The Physical Process Validation is using the numerical model to simulate a series of selected laboratory experiments to determine whether the numerical model is capable of reproducing the basic physical processes, especially those of key importance to the application case. Finally, the test of the numerical model's capability of producing field behaviors of a real-life problem is to be answered by the Site/Case-Specific Validation Test.

It is believed that before selecting a numerical model to investigate a hydroscience and engineering problem of importance the model has to be tested by this or similar validation and verification process systematically.

INTRODUCTION

Computational modeling has become not only preferred, but also required research and design methodology in hydroscience and engineering recently. More and more computational models have

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been and are being developed and applied to the investigations of complex real-life flow problems in irregular domain, with a large number of multi-disciplinary effects and/or forcings covering a large area and for long periods of time. These projects often cost large sums of funds and have long term economic, ecological and environmental impact. Therefore, a high level of accuracy and reliability of the predictive tools has been increasingly demanded.

The American Society of Civil Engineers (ASCE) and its division, the Environment and Water Resources Institute (EWRI) have established a task committee on three-dimensional free surface flow model verification and validation since early 1990's to develop a comprehensive procedure for both model developers and users to verify the correctness in mathematics and validate the capability in reproducing the physical characteristics and processes of free surface flow phenomena. Most of the findings reported in this paper are the result from this task committee with the author serving as the chair. The valuable contributions of committee members from six countries leading in hydroscience and engineering modeling research are sincerely acknowledged. The detailed information is being edited in an ASCE Monograph (wang, et.al. 2006) to be published.

HYDROSCIENCE AND ENGINEERING RESEARCH

Better understanding of water flows and more effective utilization of water resources have been the motivation to advance the state of the art of hydroscience and engineering. By observations and measurements of water movements in nature, basic physical principles and laws have been hypothesized. Subsequently, they have been subsequently described by mathematical equations and functions and proven by carefully conducted experiments in the laboratories. Even though these basic laws and principles are often proven only under highly idealized assumptions and simplifications, they have, nevertheless, established the foundation of our understanding of hydrosciences.

In another significant development, mathematical modeling methodologies have been successfully applied to describe how water flows and explain why it moves. The greatness of early philosophers, mathematicians and scientists was in their ability to idealize the hopelessly complex and seemingly random water movements in nature into simplified mathematical models, which can be solved analytically. The analytic solutions of the highly simplified mathematical models have provided us with the capability to predict hydro-systems' responses to various external forcings, at least under the idealized assumptions. The predictive capability has opened the door of a mathematically based hydro-engineering. The beauty of the nature is the fact that the simplest models are capable of capturing her most fundamental behaviors.

The need of better understanding of more realistic natural and man-made hydro-systems has accelerated the advancement of hydroscience and engineering research using more and more sophisticated field monitoring, laboratory experimentation, and mathematical modeling. More realistic physical systems usually require nonlinear differential equations to represent. The state of the art of nonlinear differential equations has yet been advanced to the level that one can systematically obtain the analytic solution of a set of general nonlinear differential equations. As a result, the scaled physical modeling has been used as the primarily tool to confirm the effectiveness of hydraulic engineering designs and constructions for decades.

As the hydrosystems become more and more complex involving multidisciplinary consideration and cost-effective optimization under ecol-environmental and other constraints, the physical modeling methodology has become ineffective and impractical. Because many tests are required to determine the optimal values of a large number of design parameters; the scaled physical modeling technique has been found to be just too costly and time-consuming to use. Therefore, the Computational Modeling methodology has been utilized by more and more hydraulic engineers to assist, and in some cases, even to substitute the physical modeling for carrying out the engineering designs. For similar reason, it has been also applied to hydroscience research.

COMPUTATIONAL MODELING

With the availability of newly advanced numerical solution methodologies and powerful computer technology, the mathematical models of nonlinear, realistic hydrosystems have been solved by numerical methods such FDM, FEM, FVM, etc. Additional computational and information science and technologies, such as GIS (Geographic Information System), GUI (Graphic User Interface), Scientific Visualization, Vistual Reality Display, etc. have been applied to the development of pre- and post-processors of computational simulation models. The resulting software packages have been not only powerful and user-friendly; but also efficient and cost-effective.

As a result, more and more computational simulation models have been developed and applied to the hydroscience and engineering research and design. Lately, some of these models have also been applied to the decision making in planning and management. It is not surprised that computational modeling has been the methodology of choice of hydraulic engineers as well as hydroscience researchers. It has been even called the research and engineering tool of the 21st century.

ACCURACY AND RELIABILITY

Due to the popularity, a large number of computational simulation models have been developed. After some simple or heuristic mathematical testings of models' accuracy and by comparing the numerical solutions to the laboratory measurements or limited field data to confirm their capability in predicting physical phenomena, these models were put on the market. Complaints about their inadequate capability and inaccurate results are abundant. Professionals in the field, hydraulic research institutions and professional societies have initiated various efforts trying to establish some standards for maintaining a reasonable level of accuracy and reliability of the computational models, or at least to provide the prospective users a means to test the capability, accuracy and reliability before they adopt a model for application to projects, especially for those major ones costing huge sums of monies and having long-term impact on our society.

This paper is to present one of these findings resulted from the intensive studies of the ASCE-EWRI Task Committee on 3D Free Surface Flow Model Verification and Validation.

A SYSTEMATIC MODEL VERIFICATION AND VALIDATION PROCEDURE

After a numerical model has been developed, it should be mathematically verified first by using at least a chosen analytic solutions, or prescribed or manufactured solutions for a linear or nonlinear case. Once the model is proven mathematically correct, it should be evaluated through a physical process validation step. At this step, one or more test cases based on laboratory experimental results should be evaluated to determine whether the model is capable of reproducing the basic physical processes relevant to the physical problems to be studied using the model. These two basic tests may be conducted once for each model. Once a numerical model satisfies these two basic test steps, it is confirmed to be free of mistakes mathematically and capable of reproducing basic and relevant physical processes. These two fundamental steps need to be repeated, however; whenever this model has been upgraded with major changes to either the physics represented or the numerical methodology. The second step needs to be conducted again, if the model, even without upgrades, but is to be applied to study a new problem requiring capabilities of reproducing additional basic physical processes.

Before a numerical model is to be applied to an investigation of a real-world problem, one more step, the Application Case & Site-Specific Validation, is required. Before this step is to be carried out, the tester is suggested to use an appropriate portion of field data collected at the study site to calibrate the site specific values of the model parameters. Then, the calibrated model is used to predict field characteristics and processes under prescribed forcing, and the predicted results are compared with those measured data at the same site under the same forcing conditions. If a reasonable agreement between the model simulations and the field measurements is achieved, the numerical model is validated only for the application to the study case at the specific site. During the validation test(s), it is very important that the calibrated model parameters can not be changed or tuned. One is not recommended to apply this model to the study of a similar problem at a different site, nor a different case at the same site, especially at a significantly lapse of time, e.g., a few years later or for a different event. To conduct an application case and site-specific validation successfully, one must have a sufficient amount of high quality field data collected at well-designed locations with proper spatial distribution. The users are reminded that it is more important to calibrate the values of model parameters to achieve a reasonable over-all accuracy of most of the measured data in the entire study domain, than to achieve highly accurate agreements at a small number of selected data points. Due to the fact that the numerical model represents a highly idealized and simplified system of the real-life problem, which is quite different from the highly complex real-life system with influences of a large number of not measured forcings, spending a tremendous amount of effort to achieve a near perfect agreement between the results of the two somewhat different systems at a few data points by tuning the model parameters, sometimes locally, is not necessary. For the same reason, the predictions of the correct trends of the spatial and temporal variations of field properties of the system being studied are more important than the accurate magnitudes of the field variables themselves. From the discussions above, one may begin to realize the fact that a numerical (or similarly, a physical) model is almost impossible to be comprehensively validated from the application point of view. Therefore, this third step, application case and site-specific validation needs to be conducted for each application site on a case to case basis.

Furthermore, it is recommended that a Grid Convergence Test is performed as the last test of the third step. It can reconfirm that with all numerical errors during the actual calculations in an application, and that the model results' accuracy is improved as the grid is refined. This test can be conducted by reducing the grid spacing (or doubling the number of grid nodes along each axis of the discretized domain). It may take some time and computational effort, but it is worthwhile for building the confidence in the results' accuracy and reliability. The reader needs to make sure, however, that to make a grid refinement test special, care has to be made during the grid refinement process, so that the physics of the model is not changed. This means that the model's bathymetry and all boundary conditions should not be changed during the grid refinement process.

CONCLUDING REMARKS

Both model developers and users are highly recommended to use the systematic procedure presented to verify and validate the model they are developing or planning to apply. The model users without the access of the source code may need the model developer's assistance in conducting the Mathematical Verification. Sometimes, the results of the mathematical verification may have been documented by the developers. In these cases, the user can request a copy of the document. Similarly, if the Physical Process Validations may also have been conducted and documented by the model developers. If this is the case, the mode user may just refer to it, rather than conducting the test again. If the user plans to use both physical and computational modeling to carry out the investigation, she/he should conduct a Physical Processes Validation to compare the measured physical data to the computational simulation results. If the discrepancy especially in trend is non-negligible, he/she may want to request the model developer to correct or improve the model or to test a different model. The Application Case and Site-Specific Validation are highly recommended to be conducted by the user before deciding to adopt a model for application. It is highly recommended that a sufficient amount of reliable field data at the study site is extremely important, because it is directly related to the accuracy and reliability of the computational simulation results. In order to collect sufficient amounts of field data at a reasonable cost, one may want to run some preliminary computational simulations to understand the flowfield characteristics, from these results, the distribution of the density and locations of the measuring stations can be chosen more intelligently to gain cost-effectiveness. A Grid Convergence Test is needed to verify that the calculation errors are reducing when the grid is being refined. The knowledge gained from this test can be used to select the grid sizes and their distributions over the entire computational domain to achieve the required accuracy at least computational cost during the production runs. This may be referred to as the grid optimization. During grid optimization process, the model user can use the real bathymetric and boundary conditions at the newly identified boundary nodes to gain higher accuracy, because the model has satisfied all verification and validation tests.

The model developers should conduct this systematic Verification and Validation Procedure as comprehensively as possible to insure that the model developed shall be free of all possible mistakes and/or errors as one can anticipate, and to make sure that the model is as capable as it can be in applications to a series of related real-world problems under various forcings and boundary conditions. The models' Verification and Physical Process Validation results should be documented and made available to the prospective users. Additional features should be built into the model, which facilitate the prospective model users to conduct the Mathematical Verification, Physical Process Validation, and even Application Case and Site-Specific Validation conveniently without the need of the source code of the model.

It is firmly believed that the application of the proposed verification and validation procedure shall greatly enhance the accuracy and reliability of the computational models and the utilization of the verified and validated computational models can accelerate the advancement of the forefront of the state of the art in computational hydroscience and engineering.

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