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ON THE DEVELOPMENT OF AN INTELLIGENT CODE VALIDATION SYSTEM FOR THE RAPID TRANSFER OF TURBULENCE MODEL TECHNOLOGY

P. G. Huang and J. D. Jacob
Department of Mechanical Engineering
University of Kentucky
Lexington, KY 40506-0108
E-mail: ghuang@engr.uky.edu, jdjacob@engr.uky.edu

ABSTRACT

Issues related to the development of a Code Validation System (CVS) are presented for the rapid transfer of turbulence models in Computational Fluid Dynamics (CFD) to industry and research. While CFD has become a successful and critical tool in many industries in both application and R&D, it has not kept pace with the progress made by turbulence models. This is due primarily to the inefficient and crude method of transfer of newly developed turbulence models to the CFD community. Timely transfer of this critical knowledge would help ensure that industry and government research scientists keep pace with current trends and progress made by turbulence modelers. Design considerations related to the development of a turbulence modeling information data base, or CVS, are presented that will bring together turbulence models, numerical algorithms, and experimental data and transfer this information via the Internet and World Wide Web to developers and end-users of CFD codes allowing proper use of the latest models and inherent their limitations.

INTRODUCTION

Background

Despite the significant advances of Computational Fluid Dynamics (CFD) in recent years, turbulence modeling is still critical to its success for most applications. As commercial CFD software products become widely available that offer user friendly but not necessarily more accurate solutions to fluids problem, the question of validation becomes increasingly important. As many engineers not specifically trained in fluid dynamics are not aware that laminar solutions are the exception and that turbulence remains an outstanding difficulty in this field (e.g., Bradshaw, 1994; Gharib, 1996), the amount of trust in the accuracy of these solutions is often greater than it should be. This results in an increased margin of error that may not be worth the reduction in computational costs. This is particularly true in the field of aerodynamics, where the margin of error is typically more critical than in industrial cases. A successful CFD tool would enhance our understanding of the effects of viscous, high Reynolds number flows associated with the innovation of future conceptual designs whose performance requirements are pushing the envelope of our experience and for which “time to market” considerations are requiring more sophisticated CFD early in the design cycle. Arguably, the three-dimensional time-dependent solution of the Navier-Stokes equations could provide an exact description of the turbulent motion, but the range of time and length scales associated with turbulence are such that they cannot be resolved when computing complex turbulent flows. As a consequence, the Reynolds averaged form of the Navier-Stokes equations together with a turbulence model are the most practical means today of computing complex aerodynamic flows.

Development of turbulence models used in Reynolds averaged Navier-Stokes (RANS) codes has been evolutionary and the resulting pace has frustrated the CFD community. Factors influencing this attitude include several aspects:

- The number of modeling research and development studies have proliferated over the last decade, yet no clear choices among suitable models seem to be emerging.

- The test cases used to validate turbulence models are often only weakly relevant to the "real" flow applications.
- Reported successes are frequently fragmentary or inconsistent and the numerical aspects and their impact on efficiency are rarely discussed.
- There is a general lack of a systematic effort to transport a "successful" model into CFD application codes.

All of these items continue to exacerbate the situation and enhance outsider's perceptions that the process for selection of a model is Byzantine and inefficient.

There is little doubt that there has been significant progress in the field of turbulence modeling research in the last decade, especially considering the fact that we are dealing with a very difficult problem. Although the growth in the field of turbulence modeling research is very much in parallel to that of CFD research, there is a fundamental difference between the two areas – CFD is gradually evolving into a mature science while turbulence modeling is still in its infancy; many modelers are still trying to find the universal model. Industry has started to use CFD technology for their design purposes, even though the physical models used in most of their CFD codes are less than satisfactory.

In the development of CFD tools, a general consensus is to reduce the number of application codes; the code developers are then encouraged to build new modifications on the existing codes. This not only ensures continuity for engineers in applying CFD technology in engineering designs but also eliminates the unnecessary confusion that arises from the need to select the codes. On the other hand, if we were to recognize that there is no universal turbulence model available, such a strategy may not be practical. Instead, one should propose a mechanism that will allow the selection, filtering and then transfer of the good models (or modifications to the models) to the CFD developers in a timely fashion.

There is clearly a lack of this kind of mechanism between turbulence modelers and CFD developers. Historically, modeling and CFD development have often proceeded along independent albeit parallel paths. Modelers developed new or improved models demonstrated on isolated test flows that are often not as complex as those undertaken in realistic applications. Modelers then expect the CFD groups to pick and choose among the myriad of choices until the development of the universal model. When application results are less than satisfactory confusion and frustration comes to the forefront, typically at the hands of a CFD non-specialist or application engineer.

Furthermore, a general trend in aerospace industry is that their internal R&D budgets are shrinking and their ability to do turbulence modeling and model validation is diminishing, while the demands to use CFD as a tool in testing new designs and concepts are increasing. Related to this is the continuing decrease of computing costs allowing more and more complex fluid flow problems to be investigated using CFD. Figure 1 illustrates this. Experimental analysis is still preferable for highly complex systems or large amounts of data, but the point of cost equality is being extended as computers become faster and cheaper and the costs associated with experimental setups tend to remain flat or even increase. In fact, the most effective driver for CFD may be the commercial user rather than the aerospace sector (Cosner, 1997). The caveat associated with this is that CFD is notorious in incorrectly predicting complex flow physics without rigorous validation tests. Thus, the relative ease and cheapness of using CFD may be a disadvantage rather than a benefit to the fluids community.

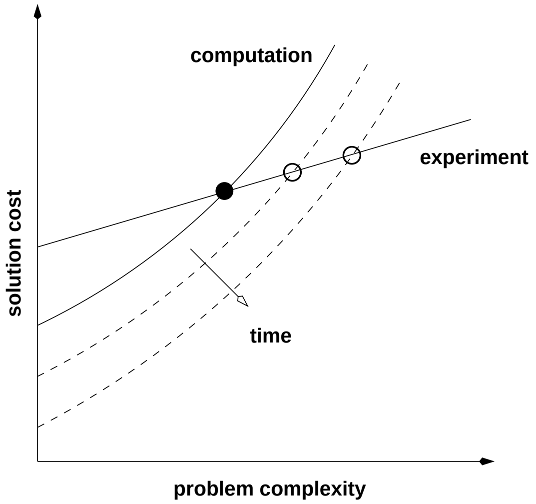

Figure 1. Comparative relationship between costs of experiments and costs of computations to solve a particular problem. As computing costs decrease over time, the cost-allowable complexity of problems solvable by numerical simulation increases. (Adapted from Rubbert, 1990.)

In view of this situation, a more collective effort, over seen by members of the CFD community, including algorithm developers, turbulence modelers and experimentalists from industry, academia, and government laboratories, through a "living" information system, with an aim to resolve the issues of turbulence modeling in a more and organized fashion is necessary. The obvious medium for this effort is the Internet, specifically the World Wide Web (WWW), whose multi-media nature lends itself well to collaboration among distanced researchers.

In order to ensure that the CFD codes developed for various applications use the best available modeling and to ensure that the model implementations are correctly carried out, the new paradigm of model development proposed by Marvin and Huang (1996) will be used as the base development principle for this project. This paradigm is illustrated in figure 2, where the gap between fundamental test cases and complex industrial applications is closed.

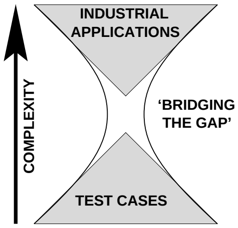

Figure 2. Traditional test cases tend to be too simple to be useful to industry. More complicated cases need to be tested and made available to bridge the gap.

Objectives

The overall goal of this work is to empower industry and other CFD end-users to make informed decisions regarding the validity of their numerical results. Several steps are necessary to make this possible, outlined in detail below.

The first objective is to perform a comprehensive turbulence-model evaluation. This can be achieved by following closely the guidelines of the model selection process recommended by Marvin and Huang (1996), Huang (1997), and Bardina et al. (1997a, 1997b), where models are evaluated against select experimental data sets. The above papers give sample validation procedures using a number of experimental data sets and turbulence models. These data sets include four fully developed free-shear flows, an incompressible boundary layer, and three complex flows with flow separation; particular use is made of data from the 1980-81 AFOSR-HTTM-Stanford Conference on Complex Turbulent Flows (Kline et al., 1981). Turbulence models evaluated include four well known and oft-used models: the two-equation $k-\varepsilon$ of Launder and Sharma (1974), the two-equation $k-\omega$ model of Wilcox (1988), the two-equation $k-\omega$ *SST* model of Menter (1994), and the one-equation eddy-viscosity model of Spalart and Allmaras (1994). The aim is to extend the original data base by increasing the number of test problems and by covering a wider range of models, allowing evaluations that are either more narrow (by validating a single model against a specified data set) or more general (by validating a model against many varied data sets). The new test problems should also contain a few complex 2-D and generic 3-D experiments. Additional turbulence models should include higher-order linear and non-linear eddy viscosity models, 3-equation eddy viscosity models and ultimately, Reynolds stress models.

The second objective is to develop, implement, and maintain a turbulence model data base that will act as a selection and filtering mechanism to ensure that CFD codes developed employ the best available turbulence models. The data base should consist of (1) turbulence model descriptions including numerical stabilizing strategy and source-term treatment, (2) a standard experimental data base for modeling assessment, (3) studies illustrating model sensitivity to such parameters as grid spacing, first y-plus location, free stream boundary conditions, relative computational cost, etc., and (4) standard numerical solutions using various turbulence models that will allow CFD developers to verify their model implementation. The data base should be accessible through the Internet via the World Wide Web and initially limited to government agencies, research centers, and companies that have extensive need for a database such as the aerospace and gas turbine industries. This data base will comprise a Code Validation System, or CVS, which allows users to systematically evaluate the performance of CFD codes and turbulence models for a specific application.

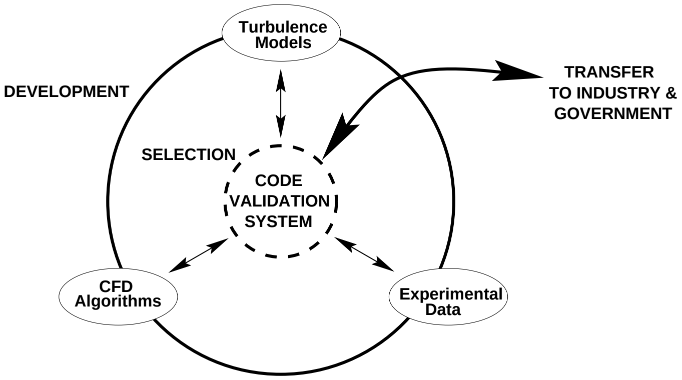

Figure 3. Conceptual diagram showing development and filtering of a database, or Code Validation System (CVS), from turbulence models, CFD algorithms, and experimental data, and transfer of this knowledge to industry via the World Wide Web.

The research will be coordinated with select personnel to form an impartial oversight committee consisting of members from government, industry and academia. The Committee will establish a set of turbulence modeling evaluation criteria or metrics that turbulence modelers would be encouraged to apply in their development process. These metrics would enable CFD code developers to make intelligent choices for models to incorporate into their application code and to provide modelers (and the fluids community at large) with relevant comparative standards to assess progress on new or improved model development and to identify shortcomings of current models.

The objective is illustrated in figure 3. Turbulence models, CFD algorithms, and experimental data are brought together in a development process to validate models and codes against experimental data. The selection process determines which codes and models should be placed in the WWW data base. These are implemented in the CVS, through which industry and government research institutions can easily determine which models best fit their current needs, or evaluate the validity of their own models. The process is transparent, i.e. end-users will be able (and encouraged) to report on the success of models and algorithms obtained from the system.

DOWN-SELECTION PROCESS

A successful CVS involves several critical components, each of which can lead to failure if not properly implemented (Marvin and Huang, 1996). These are listed as follows:

1. selection of relevant experimental data,
2. selection of turbulence models,
3. model validation and
4. technology transfer.

The first three elements have been commonly used in model development, though usually not with the rigor suggested herein due to the limited use of most models and codes. Simply displaying this list reveals that these components are inextricably linked to one another; a successful model *must* be properly verified with quality experimental data, viz. a data set for which the measurement conditions are well determined. In addition, it is also important that the computational accuracy be assessed. All experimental and numerical errors must be known. This cannot be understated. The last element, technology transfer, is perhaps the most challenging as it has not been previously accomplished; it is certainly the most important for a successful CVS as it is the crux of the development process presented herein.

Experimental Data Base

A range of pathological test problems has been previously recommended (Marvin and Huang, 1996; Bardina et al., 1997a). These cases consist of several free shear flows and a number of complicated but relevant 2-D flows. These are selected based upon the paradigm presented in figure 2. Simple test cases are selected for both external and internal flows for preliminary model validation. The complexity of the physics of the test cases, hence the complexity of the solutions, increases as more cases are validated. Thus, a code intended for general use can be given some value of accuracy with respect to several complex flow solutions.

Experimental data sets of flows for a successful CVS are suggested as follows:

1. External flows
   - *(a) Incompressible flat plate boundary layer*
   - *(b) Adverse pressure gradient flow*
   - *(c) Self-similar mixing layer*
   - *(d) Self-similar round jet*
   - *(e) Self-similar plane jet*
   - *(f) Self-similar plane wake*
   - *(g) Compressible boundary layer*
   - *(h) Compressible mixing layer*
   - *(i) Transonic bump flow*
2. Internal flows
   - *(a) Flow over a backward facing step*
   - *(b) Sudden pipe expansion*
   - *(c) Single annular jet in a rectangular test section*
   - *(d) Coaxial jet*
   - *(e) Single swirler with no corner expansion*
   - *(f) Shrouded swirler*
   - *(g) Impinging jet; plane and inclined*
   - *(h) Impinging vortex ring*
   - *(i) Boundary layer flow due to convex curvature*

These cases build upon the initial flow data base recommended by the NASA Standards Committee needed to facilitate interaction between modelers and CFD code developers. These experimental data sets reflect a vast range of physical parameters ranging from basic flow physics to complex configurations and yield a wide array of metrics that will help bridge the gap between model testing and industrial model application. Particular emphasis will be placed on selecting superior experimental data and well specified boundary conditions the lack of which would plague any stringent validation procedure. Additional external and internal test flows should be added to generalize the data base, especially with data from the 1968 AFOSR-IFP Stanford Conference on Turbulent Boundary Layers (Kline et al, 1969), the 1969 (Bertram, 1969) and 1972 (NASA, 1972) NASA Conferences on Compressible Turbulent Boundary Layers and Free Shear Flows, respectively, and most notably, the 1980-1981 AFOSR-HTTM Stanford Conference on Complex Turbulent Flows (Kline et al., 1981).

Validation is the first, but not only, measure of model goodness. Generally, the wider range of flow examples contained in a CVS, the wider possible use of a validated model in flow calculations.

Turbulence Models

Turbulence models can be of many types ranging from 0-equation to complicated multi-equation Reynolds stress models. While simpler models are popular among CFD code developers, complicated models provide better modeling physics and, arguably, are more likely to be successful in a wider range of flows. However, to what extent an advanced model can improve the solution is generally not well defined. In addition, experience shows that the solution of higher order turbulence models is typically not straightforward. The numerical strategy involved to stabilize a particular model and the efforts needed to port a particular model into application codes are generally not reported by researchers. In this study, the emphasis will be focused on the definition of the models' success and failure in different benchmark flows and the documentation of numerical stabilizing strategy of various selected models. It may also be beneficial to have a model classification scheme based upon various model parameters such as that presented in Bardina et al. (1997a).

Model selections for a successful CVS are suggested as follows:

1. Launder-Sharma $k-\varepsilon$ model (1972, 1974)

2. Wilcox $k-\omega$ model (1988)
3. Menter SST model (1994)
4. Spalart-Allmaras 1-equation model (1994)
5. Reynolds stress models
   (a) Launder, Reece and Rodi (1975)
   (b) Shih and Lumley (1985)
   (c) Speziale, Sarkar and Gatski (1991)
6. Non-linear models
   (a) Fu, Launder, and Tselepidakis (1987)
   (b) Gatski and Speziale (1993)
   (c) Shih and Lumley (1995)
7. 3-equation eddy viscosity model of Durbin (1995)

Additional models should be tested and implemented as they become publicly available. Thus, an ideal CVS would be a clearinghouse listing of currently available models and their inherent benefits and disadvantages. This would greatly reduce the time it takes to determine which model would be best suited for a particular application. In the future, a CVS may even be used as a proving ground to test turbulence models, aiding turbulence modelers in developing new models more quickly and accurately.

Model Validation Procedure

Experimental Data Validation requires detailed knowledge of the experimental data and how they were obtained. This includes such things as whether the measurements were time-averaged or instantaneous, the error of the measurement technique (viz., accuracy and precision), detailed information about the geometry including effects of three-dimensionality, and initial and boundary conditions. Thus, for the data to be at all useful for validation, it must be well documented. The type of measurements are also important, including which quantities are directly measured and which are derived. Once these items have been determined, then it is possible to make a measure of the overall usefulness of the data in possible validation. This is somewhat subjective, but the end goal is to verify the ability of a model to predict flow physics, not assess individual data quality. Before using any data in validation, one must be absolutely confidant in its accuracy and should be able to answer the following question: "how well does the data compare to other experiments investigating similar flows?"

Sensitivity Tests Model validation can be tedious. In addition to comparison with requisite experimental data sets, it involves many sensitivity tests, such as grid refinement, placement of the first y^+ location, free stream boundary conditions, code dependence, etc. (Marvin and Huang, 1996; Huang, 1997; Bardina et al., 1997a). Several of the most important tests which should as the primary sensitivity tests in a CVS are discussed here. A grid sensitivity study for each turbulence model is used to provide an indication of how fine a grid must be to obtain an accurate solution. This is not only helpful in this respect, but it aids in keeping the grid from being too fine and using unneeded computer resources. Related to this is the sensitivity of the location of the first grid point from the wall. This is especially important in boundary layer flows where relevant physics may be lost. Free-stream and inlet conditions account for the level of turbulence and ratio of viscous to inertial effects. Similarly, the importance of compressibility effects must be determined. Lastly, it must be established that the model solutions are code independent as well, allowing them to be transferred from code to code without affecting the result. This is particularly important since many codes use different physical simplifications. A list of the six suggested primary sensitivity tests and their requisite parameters is given in table 1.

Sensitivity Test	**Parameter**
Grid Resolution	Number of grid points
y_i^+	First point from wall
Free-stream Conditions	Turbulent viscosity
Inlet Conditions	Reynolds number
Compressibility	Mach number
Code Invariance	Numerical algorithm

Table 1. Possible sensitivity tests and their associated parameters.

Future research effort should be devoted to carefully assessing these aspects. The outcome will not only serve as a guide for the choice of the suitable models for CFD predictions, but will also provide useful guidelines for CFD code developers in implementing and ultimately calculating more complex systems.

These are only a few of the many possible validation parameters. As the CVS progresses, tests may include additional sensitivity parameters or other metrics. Regardless, any validation procedure should be well documented.

Measure of Goodness To help CFD developers and engineers choose the best model for their system, a measure of model goodness or trust is required. Ideally, this measurement would include results from validation runs against experimental cases, all sensitivity tests, performance costs, and ease of implementation. Each category would be given a numerical score whose weight would apply in determining an overall score of model goodness. Such a global ranking system, while having the benefit of a simple final measure, may be misleading as to the effectiveness of a model in certain applications, however. Thus, each measure must be accompanied by several caveats.

A sample measure is shown in tables 2 and 3 with model

Test Case	Model $k-\omega$	$k-\varepsilon$	S-A	SST
Mixing Layer	1	5	5	5
Far Wake	1	2	5	2
Plane Jet	1	5	2	5
Round Jet	1	4	1	4
ZPG BL	5	5	5	5
APG BL	2	1	4	5
Trans. Bump	2	1	3	4
RAE 2822	2	1	3	4
Average	1.9	3.0	3.5	4.3

Table 2. Sample model scoring: validation. Validation is not only important in determining which models work well for a specific flow, but also which models perform the best overall.

Sensitivity Test	Model $k-\omega$	$k-\varepsilon$	S-A	SST
Grid Resolution	4	3	4	3
y_1^+ Spacing	3	1	4	3
Turbulence Level	1	5	5	5
Angle-of-Attack	4	4	4	4
Inlet Profiles	5	5	5	5
Numerical Code	4	4	4	4
Average	3.5	3.5	4.3	4.0

Table 3. Sample model scoring: sensitivity. Sensitivity scores show how well a model performs under varying implementation parameters. Note that equal average scores do not mean that a models perform identically in all tests. For proper model selection, the details are important.

performance and sensitivity results from Bardina et al. (1997b). Each model is given a performance score from 1 (poor) to 5 (good). Though each model's score in each area is easily calculated (every system is admittedly arbitrary to some degree, but relative scores between the represented models is what is important), the results can be deceiving, particularly when a final overall score is desired. E.g., in the scores given if the model validation and sensitivity tests are equally weighted, then the SST model appears to perform the best. Equal weights may not be preferred, however, if one model validation is considered less important than another. This is important where a solution for a specific geometry is required rather than a general solver, for example Thus, if the validation and sensitivity tests are weighted with 25% and 75% factors, respectively, then the Spalart-Allmaras model obtains the highest score. Also, the final rankings may be misleading as they do not take into account coordinate variance in these tests, where the $k-\omega$ and $k-\varepsilon$ models perform well but the S-A and SST models do not. If this area is particularly important to the CFD engineer, then the scores become meaningless.

This is only one example of the complexity of assigning a measure of goodness. Thus, it is unlikely that a single numerical value can be attached to a model to evaluate its overall performance. However, a few values, with requisite caveats, should be sufficient to evaluate a model's goodness for all but the most rigorous of users.

Technology Transfer

The last, but certainly not the least, effort of this research is to transport the know-how to CFD code developers and application engineers. This would involve the use of the Internet through the WWW (Marvin and Huang, 1997). The resulting data base would employ current WWW technology such as Java to allow the end-user to manipulate the system's parameters in real time WYSIWYG. Basic structure of a CVS is shown in figure 4. At its core, the system consists of the CVS data base containing the experimental data sets, turbulence models, and sensitivity tests, including a number of numerical codes. A CFD engineer or code developer accesses this system through the WWW and the CVS oversight team. The team, whose main task is to oversee the smooth operation of the CVS, administers jobs submitted to the CVS as well as implementing improvements into the data base. Results from a submitted job taking the form of a goodness score or some other measure are reported back to the CFD engineer who can then use this information to his benefit or pass it on to other users. Typically, the system would contain such information as model descriptions, numerical strategies for solving the model equations, the standard data base, and the standard numerical solutions. A CVS will serve as a vehicle for communication among experimentalists, CFD code developers, and modelers.

RESOURCES AND IMPLEMENTATION

A successful CVS calls for relatively small expenditures on hardware, with the purchase and maintenance of a workstation to operate as the CVS WWW server and data base being the only major hardware item. If significant testing and evaluation is being performed, either by the CVS oversight team or by CVS users, then an additional workstation is desirable to ease the load on the WWW server. The Internet connection speed largely depends on the type of results sent back to a CVS user. A simple good-

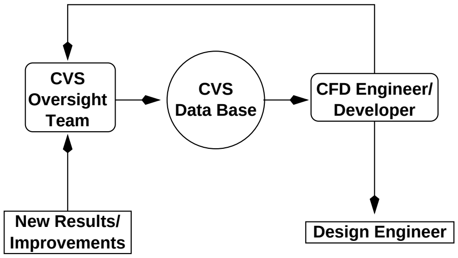

Figure 4. Flowchart of technology transfer of turbulence models using a CVS. The system should allow for feedback, valuable for determining effectiveness of data and improving the validation procedure.

ness score, even with many caveats, would require the simplest of lines. However, if numerous graphical or tabular CVS results from model test and validation are required, then ISDN, T1, or faster connections are desirable. The size of the CVS oversight team depends largely upon the responsibilities given them and the number and type of CVS users/customers. Ideally, a team would consist of a leader whose responsibilities include CVS mission management and team supervision, and several CFD coders and turbulence modelers to work on the running of submitted jobs and implementation of new results. Once a CVS is fully automated, then the oversight team's tasks are reduced to the latter item. It is vital that the oversight team have links to researchers in the field, both those developing new models and those implementing them. This ensures that the latest models are fed into the CVS data base and that feedback on CVS performance is received and timely tuned.

Figure 5 shows a CVS under development at the University of Kentucky. The site allows users to choose an experimental data set which most resembles their flow characteristics and a turbulence model(s). For previously validated models, standard solutions and scores are then supplied from the data base. The use can then use this information along with online comments of how to properly implement the selected model in his software and apply this directly to the problem-at-hand. If the specific combination selected has not yet been validated, then the job can be submitted or downloaded to perform a full validation and scoring. In addition, new turbulence models can be submitted for evaluation. The results will then be made available to the submitting and other CVS users once screened by the oversight committee. New data can be submitted in a similar fashion. Thus, the database continually grows to match its user base. Once the system is fully automated, the CVS should be able to make recommendations about which model to use for a given flow.

SIGNIFICANCE AND IMPACT

Timely technology transfer between turbulence modelers and CFD code developers has not been satisfactory. This proposed selection process will guarantee that the codes developed for fluid flow applications use the best available turbulence models considering trade-offs between computational efficiency and accuracy of physical modeling. Furthermore, it will ensure that the models are implemented correctly in the CFD codes so as to eliminate errors due to improper handling of aspects of grid and numerical and boundary conditions. This can greatly reduce the time and cost of model implementation while increasing the accuracy of and trust in numerical results. This is a necessary step in the ongoing metamorphosis of CFD from an emerging to a mature technology.

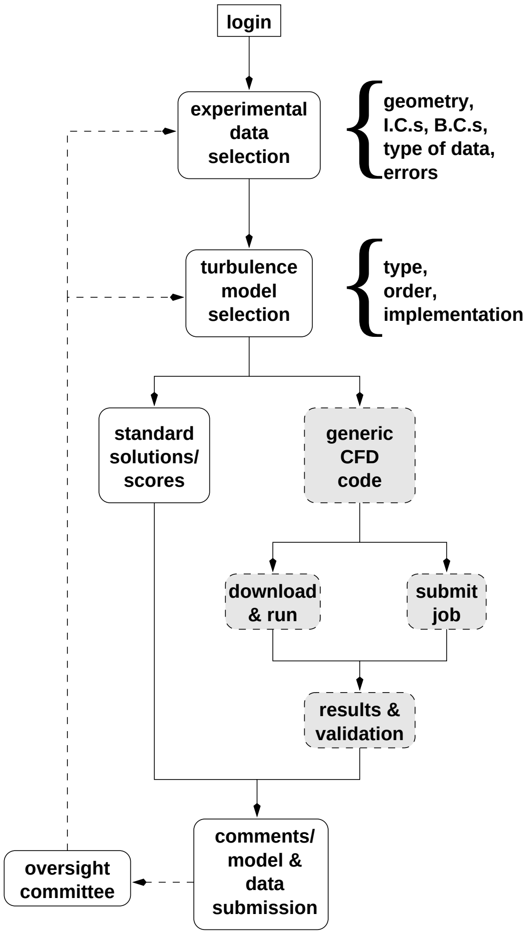

Figure 5. Flowchart of CVS site. The first version (simplest) follows the left path. Little of the system is automated and results are limited to tests performed a priori. Shaded boxes show the automated system where users can mix and match models and data.

CONCLUDING REMARKS

Simulations have become an increasingly popular commodity to the industrial community-at-large for many reasons, but while CFD has become a successful and critical tool in both application and R&D, it has not kept pace with the progress made by turbulence models. Timely transfer of this critical knowledge would help ensure that industry and government research scientists keep pace with current trends and progress made by turbulence modelers. The CVS as presented herein will bring together turbulence models, numerical algorithms, and experimental data, and transfer this information via the Internet and WWW allowing end-users of CFD codes to properly use the latest models and understand their limitations. Development of such a system is a necessary part of the greater evolution of CFD into a reliable technology for day-to-day engineering use. Agencies or persons planning on establishing a CVS should take many parameters into consideration, only some of which are presented herein. Above all, the CVS should aid in model selection and the overall goal of improving the process and results of numerical simulations should not be lost sight of.

Using the suggested guidelines discussed herein, a prototype version of an intelligent CVS, named *CoVaS*, is being constructed at the University of Kentucky and will be available for testing. Because of the sensitivity of the data base, initial access will be controlled by the University of Kentucky and restricted to selected research agencies and industrial offices.

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