International Journal of Advances in Engineering Research http://www.ijaer.com

(IJAER) 2015, Vol. No. 10, Issue No. III, September **e-ISSN: 2231-5152/ p-ISSN: 2454-1796**

COMPUTATIONAL MODELING FOR RESEARCH AND DEVELOPMENT: TOOLS AND TRENDS

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ABSTRACT

The exponential growth of computing performance was also combined with the increasing availability of large scale computing resources, for the benefit of the Computational Fluid Dynamics (CFD) research and most commercial software providers are up-scaling the software potential to serve the user base. In this article some available commercial software's for CFD research are introduced and the importance of the necessary steps of verification and validation are emphasized.

Keywords—Simulations; CFD; Research; Verfication; Validation

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INTRODUCTION

The development of the whole discipline of fluid dynamics is evolving with time. The basic foundations of experimental fluid dynamics were laid in France and England, during the seventeenth century. Following, gradual development of theoretical fluid dynamics was observed in eighteenth and nineteenth centuries. The study and the practice of fluid dynamics, for most of the twentieth century, involved the use of pure theory on the one hand and pure experiment on the other hand. The advent of the high speed digital computer combined with the development of accurate numerical algorithms for solving physical problems on the computers has revolutionized the way we study and practice fluid dynamics today. It has introduced an important new third approach in fluid dynamics- the approach of *Computational Fluid Dynamics* (CFD) [1].

In today's world CFD is an equal partner with pure theory and experiment in the analysis and solution of fluid dynamics problems. CFD is simply a new approach-but nothing more than that. It nicely complements the other approaches, pure theory and pure experiment, but will never replace either of these approaches. Fluid flow and related phenomena can be described by partial differential equations, which cannot be solved analytically except in special cases.

In CFD, to obtain an approximate solution numerically, a *discretization method* is used which approximates the differential equations by a system of algebraic equations, which are then solved on a computer. The approximations are applied to small domains in space and/or time so the numerical solution provides results at discrete locations in space and time. When the governing equations are known accurately solution of any desired accuracy can be achieved in principle. However, for many phenomena (*e.g.*, turbulence, combustion, and multiphase flow) the exact equations are either not available or numerical solution is not feasible [1]. This makes introduction of models a necessity. Even if we solve equations exactly, the solution might not be a correct representation of reality. In order to *validate* the models, we have to rely on experimental data. The level of accuracy needed to solve the equations and the necessary step of validation is case dependent. While many users rely on the codes developed in-house, most industrial user base extensively relies on the commercially available software packages.

CFD COMMERCIAL SOFTWARE

Many commercial CFD softwares were developed in the last few decades and the user community is strongly growing. For example ANSYS FLUENT [2, 3], CD-Adapco STAR-CCM+ [4], Exa PowerFLOW [5]. ANSYS Fluent software contains the capabilities needed to model fluid flow, turbulence, heat transfer, and reactions for industrial scale equipment. To date there were many successful demonstrations, such as combustion phenomena in coal furnaces, resolving the flow-chemistry interactions in internal combustion engines and air flow over an aircraft wing. The software is also successfully applied to many multiphase flows, which are common in many industrial applications. STAR-CCM+ provides an environment for solving problems involving fluid/solid flow, heat transfer and stress. While EXA Corporation has developed many softwares the website describes the POWERFLOW as a software that is capable of simulating some of the world's most complex fluid flow problems. The software primarily built on transient Lattice Boltzmann technology and to capture the complicated geometric features, PowerFLOW uses advanced methodologies such as, immersive grid technology and automatic fluid grid [5].

While many of the commercial codes are verified with respect to the numerical accuracy of different solvers, it is the primary responsibility of the end user to appropriately utilize the features of the softwares. Typically the end user of these simulation tools should perform verification and validation studies before making predictions in the design space where the experimental data is unavailable.

VERIFICATION AND VALIDATION

Verification seeks to answer the question of whether the equations that compose the mathematical model are being solved correctly, and quantify or estimate the error resulting from the computational implementation of that mathematical model; it does not answer the question of whether the equations can be used to accurately describe physical reality. Verification has two separate but equally important parts, code verification and solution verification.

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Code verification is intended to accomplish two goals: first, to ensure that the implementation of the mathematical model is free of mistakes, and second, to use exact solutions to quantify the discretization error associated with the implemented discrete operators, and verify that they exhibit expected behavior. Solution verification has the goal of estimating numerical error in the intended use regime, leading to results that are more directly applicable, but it also eliminates the availability of exact solutions. Because exact solutions are unavailable, solution verification quantifies numerical uncertainty, not numerical error.

If the numerics are implemented through operators and if they are verified for accuracy, the user can simply perform the solution verification. For example if the user like to use a second order spatial discretization and third order explicit Runge-kutta method to march the solution forward in time the implementations should be verified first. For the commercial codes since most of the implementation details are not available to the end users, the important step is to perform the solution verification.

The solution verification involves mesh and time step independent study. For the grid/mesh convergence study, simulations should be performed over different spatial resolutions and evolution of different quantities should be evaluated. Based on the observed performance of the simulation a spatial resolution should be selected. Similarly when transient flows are simulated, simulations should be exercised at different time steps and accordingly time step should be defined.

After completing the necessary verification step, the most important part of any computational modeling approach is the validation. Validation involves examining if the conceptual and computational models as implemented into the CFD code, and computational simulation agree with real world observations. The strategy is to compare simulation results with experimental data to identify and quantify error and uncertainty through. The accuracy required in the validation activities is dependent on the application, and so, the validation should be flexible enough to allow various levels of accuracy. However the validation should be performed at simple cases first before embarking on to more complicated cases. NASA recommends systematic comparison of CFD simulation results to experimental data from a set of increasingly complex cases [6].

SUMMARY

In this paper, the role of computational modeling, mainly CFD, in advancing the research and development emphasized and some commercial softwares are reviewed. In the context of simulation based science, verification and validation studies are introduced and the importance is discussed.

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