Validation Problems in Computational Fluid Mechanics

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Abstract

Recent developments in Computational Fluid Dynamics (CFD) increased interest in quantifying quality of the numerical models. One of the necessary steps is so called *code validation* procedure, assessment of a numerical simulation by comparisons between simulation results and laboratory measurements. The focus of the present review is application of modern full field experimental techniques, mostly based on the digital image analysis, in validating numerical solutions of complex flow configurations.

Keywords: fluid mechanics, validation of numerical codes, experimental mechanics

1. Introduction

With the growing capacity of computers and continuing improvement in numerical codes, the question of the accuracy of numerical solutions is of primary importance. The usefulness of the numerical solution depends on its ability to model physical problem. This is evident in the number of commercial codes available for solving almost every problem imaginable in the field and may suggest that the époque of expensive and complicated laboratory experimentation has passed. Although all would welcome such a development, the validation of the numerical results remains a concern tempering some of this optimism. Typical difficulties in obtaining credible predictions for industrial problems lead to the often encountered dilemma: Do we trust numerical simulations? Of course, this is not specific for fluid mechanics only. However, strong nonlinearities of governing fluid flow equations, inevitable model simplifications necessary to solve turbulent flow, presence of complex couplings of mechanical interactions with thermal, surface, chemical, gravitational or multibody effects create multiple sources of uncertainties and serious errors. Problem of uncertainties is often neglected if applicability of the simulation results following from more or less idealized models is limited only to global description of the investigated problem. However, there is a wide class of practical problems where knowledge of just the general behaviour of flow is not sufficient to obtain a full quantitative explanation of the phenomena. Examples include the distribution of fuel or soot in a combustion chamber, the transport of impurities in crystal growth, the propagation of pollution in fluid flow, or for small scale flow phenomena. The knowledge of some specific flow details appears to be necessary for the full control of the investigated phenomenon. Improvement in the accuracy of theoretical and numerical models and their experimental validation is an indispensable procedure in such cases. This issue seems to be especially pertinent when modelling multiphase and multi-scale phenomena.

2. Verification & Validation

During the past two decades there has been a growing interest in verification and validation (V&V) as a distinct part of computational fluid mechanics. The evidence for this increased interest is the formulation of several initiatives to establish methods of code verification (i.e. checking method and accuracy of solvers). Since beginning of the computational fluid dynamics verification of the code was an important issue. Several, so called “numerical benchmarks” appeared, the first and probably best known was given by Graham de Vahl Davis [1]. Having reference solution based on apparently accurate code (usually just using high resolution discretization) other code developers could evaluate performance and accuracy of their products. The aim of the code verification seems obvious, each numerical analysis using the same model physics should produce consistent result. Nowadays a plethora of numerical benchmarks are available covering most of the typical cases. One of them worth to mention is The ERCOFTAC Best Practice Guidelines for Industrial Computational Fluid Dynamics [2]. Generally speaking code verification should establish confidence that the mathematical model and the algorithms responsible for discrete solution are working correctly. Neither part of verification process addresses the question of the adequacy of the selected conceptual and mathematical models for representing the reality of interest. This part of the code evaluation touches the second component of the V&V abbreviation, namely code validation.

The term code validation, defined probably for the first time in early 80-ties by Boehm [3], is understood as determining the degree to which the analyzed numerical model is an accurate representation of the real world. For a long time both terms verification and validation were mixed in the computer science literature without deeper understanding differences between them. As it was underlined by Roache [4] we have to confirm not only that equations are solved correctly but what is even more important for practice that we are solving the right equations. Hence, there is an essential distinction which can be perhaps in the simplest way given defining scope of the methods used:

- the code verification is based on a mathematical analysis,
- the code validation is based on experimental outcomes.

The both V&V procedures are necessary to perform Code Qualification, the last step before applying it to solve real engineering problem. This last step is the main goal of engineering applications, as it has to compare physical model used for the validation with the real industrial configuration. Finding proper methodology to perform this practical issue is problem specific, sometimes very difficult to realize.

Here, we concentrate on the code validation issues, trying to elucidate problems with preparing proper experimental reference allowing to "validate" physics of the model. Performing code validation we may define two distinct issues:

- The first obvious one, is to construct model experiment including all expected physical ingredients of the analyzed phenomena. We still use term "model", as in the most cases it is very difficult or sometime impossible to operate with the final target of the simulations. Usually size, extreme values of parameters (temperature, gravity), accessibility of the interrogated flow region, etc, force us to mimic physical phenomena at a laboratory scale. It allows for better control of all physical conditions and to apply data acquisition methods not applicable in industrial, geophysical or space environment.
- The second issue of the code validation, namely the accuracy assessment, is not less important. Having experimental and numerical data we have to define proper methodology to find the validation metric in terms of the data accuracy and sensitivity of the analyzed model outcome to inevitable experimental errors. This part of the assessment is coupled with the first one, as it defines limits of the experimental accuracy.

3. Experimental benchmarks

With recent progress of experimental methods, introduced by digital image recording and analysis techniques, validation of numerical codes using full field experimental data became one of the most challenging research goals nowadays. In few examples we aim to demonstrate methodology and outcome of validation procedure. Hence, we show that by quantifying deformation of oscillating droplets observed under a microscope it was possible to validate importance of nonlinearity and oscillations mode coupling given by the numerical model [5]. This was only possible by introducing proper metrics when comparing numerical and experimental outcome. Simultaneous measurement of the flow and temperature fields enables a relatively easy verification of global features of experimental and numerical simulations for thermally driven flow. We have shown fine details of the flow can also be properly interpreted if the particle tracks are analyzed [6]. The discrepancy between the predicted and observed flow patterns can be minimized if an interactive trail and error procedure is used, modifying „weak" points in the thermal boundary conditions, implementing the measured temperature fields as a code input, and improving the numerical code [7]. In many engineering problems such a tedious procedure may seem to be unpractical. We can not offer any universal „golden" rule which could replace it. However, it has been found that a large improvement in quality and reliability of numerical simulation can be obtained by means of validations and tuning methodologies using information obtained from the flow visualization and full field measurements.

Unfortunately most industrial problems involve configurations and substances which are very difficult to investigate experimentally. For example in case of modelling casting problems we find that metals and metal alloys are opaque, their melting temperature is very high and their physical properties are not known precisely enough. Hence, collected data is usually not sufficiently accurate to give a definitive answer on code reliability. One possible option is to use so called *analog fluids* which are transparent and have a low melting point. Such materials are most commonly aqueous solutions of salts, which crystallize with a dendritic morphology. Some organic liquids also lend themselves favourable to this purpose. Our experience is that solving complicated problems is easier when experimental feedback is present. It is impractical and usually impossible to include all possible factors when modelling the environment numerically. Properly planned experimental benchmarks may alert one to the sensitivity of the flow to such secondary flow conditions which would otherwise be hard to predict. A brief review of experimental techniques useful for the study of heat and mass transfer problems in the flow of liquid with this objective in view given previously [8] will be discussed together with the purpose of three simple configurations allowing analysis of discrepancies between measured and calculated solidification experiments.

4. Sensitivity analysis

Finally we do hope that experimental analysis of the simplified flow configuration, supported by numerical tests, allows for better identification of parameters playing crucial role in the specific flow problem. We purpose methodology to perform sensitivity analysis of the problem, delivering information about tolerance span for the accuracy in description of boundary conditions, flow geometry, and material properties. Without sensitivity analysis it is difficult or impossible to define experimental benchmark which delivers data sufficiently accurate for the proper code validation. On the other hand sensitivity analysis in fluid mechanics can be performed only using high resolution, *exact* solutions obtained using *Direct Numerical Simulation* (DNS) solvers. These relatively new numerical method may sometimes even replace experiment. Performing reference DNS simulations, despite their huge demand of computational resources, is often essential for determining code validation experimental procedure.

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