CFD at its limits: scaling issues, uncertain data, and the user's role

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Simulation codes for Computational Fluid Dynamics (CFD) may be considered mature engineering tools today. They have stood the practicioners' test of time and are routinely used in a supportive, sometimes central, role, e.g., in the shape design of airplanes or cars or for the layout of gas turbines and internal combustion engines. Here, however, we are interested in their application in safety-critical contexts and this raises the following three more fundamental questions:

First, CFD codes are based on numerical methods for the solution of partial differential equations. These methods provide discrete computational results with flow field data associated with the nodes or cells of a computational grid and with discrete levels in time. Ideally, these numerical solutions can be proven to converge to the exact solutions of the considered equations in the limit of finer and finer computational grids and smaller time steps. In contrast, most fluid flows of practical interest are turbulent, and in CFD simulations it is generally neither possible nor of interest to resolve all details of the turbulent fluctuations. Therefore, turbulent flow CFD simulations are notoriously under-resolved relative to the smallest turbulent scale, the Kolmogoroff dissipation scale. Aren't the tools of numerical mathematics then being used way outside their regime of applicability? We discuss this question and conclude that CFD has proven to be very useful even in fully turbulent settings; yet a sound scientific basis in the sense of provably correct behavior of a CFD solver is lacking both for lack of criteria and lack of a fundamental concept that would bridge the current gap between fluid flow theory and numerical analysis.

Secondly, for solutions to the fluid flow equations to be uniquely defined one must specify appropriate initial and boundary conditions and set a number of case-specific model parameters. This raises an immediate issue in the context of safety-related flow simulations because the exact circumstances of a safety-critical accident are quite generally not known in advance. Therefore, any CFD simulation carried out in the course of a safety assessment can at best be considered as one sample out of an ensemble of infinitely many possible alternative scenarios. Thus, there is a need for solid criteria for the selection of such sample simulations. This issue is closely related to uncertainty quantification for

CFD simulations. Our contribution outlines the so-called "polynomial chaos expansions" as one possible approach to uncertainty quantification. This example will not cover all issues of practical interest in the context of safety-related CFD simulations. In practice, however, the approach can provide very valuable guidelines regarding which parameter variations should be tested in an ensemble of simulations, and how to make the most of the obtained simulation results.

Thirdly, we focus on the role of the user of a CFD simulation package and on the background knowledge which the apt user should be in command of to be in a position to deliver reliable contributions to safety assessments. Here, fire safety engineering is an excellent example for the development and usage of computational fluid dynamics (CFD) in a safety critical area. The spreading of smoke in buildings can induce quite dangerous situations very quickly. A frequently asked question reads: "How trustworthy are the results generated by a CFD program?". Yet, even with the best available code at hand, a user lacking sufficient knowledge regarding the implemented physics, adopted model simplifications, and numerical schemes employed in the CFD program will not succeed in producing reliable results. Such knowledge is, therefore, just as important for trustworthy simulations as the availability of a well-tested CFD program.

We present some examples showing in which way the user can influence the computed results. Using the well documented and freely available field model Fire Dynamics Simulator (FDS) we explain some critical numerical aspects of the implemented numerical scheme and discuss their importance for the user. We show, in particular, that trustable results require both well-tested programs and well-trained users.

Summarising we highlight three important limitations of computational fluid dynamics in the context of safety-related simulations:

1. It is not possible in everyday routine simulations to resolve all details of a flow field. As a consequence, some ways of representing the net effect of processes acting on scales smaller than the computational grid size need to be introduced. Therefore, as useful as CFD simulations have turned out to be in the engineering practice in many instances, the CFD user cannot claim to be on proven, mathematically sound grounds.

2. In assessing a given situation, safety engineers are faced with much larger uncertainties than are engineers working on some typical design or optimization problem.

3. Computational fluid dynamics codes are complex and they incorporate a broad range of knowledge from fundamental fluid mechanics via numerical mathematics to computer science. It is not possible today to prove or even accurately assess the correctness of a CFD simulation in a mathematically rigorous sense. As a consequence, any CFD code is only applicable within the range of flow scenarios for which is has been thoroughly tested and validated. Users who are not sufficiently well trained in matters of the theory and practice of CFD simulations will generally not be aware of a code's limitations. Such users may easily end up applying the code to

scenarios for which it is not designed and tested and for which it therefore may or may not produce correct results.

Full article in:

Münch, M.; Klein, R.: *CFD at its Limits: Scaling Issues, UncertainData, and the User's Role*. J. Schmidt (ed.), *Process and Plant Safety, Applying Computational Fluid Dynamics*, 12, 189 – 212. Wiley-VCH Verlag GmbH & Co. KGaA, 1. Edition, April 2012.