Importance of accuracy in CFD simulations

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ABSTRACT

The application of CFD is rapidly expanding with the growth in affordability of computational resources. It is becoming essential for CFD solvers to provide validation and verification. Mesh related issues play a very important role on accuracy and convergence. The means to achieve high fidelity computational simulations of fluid dynamic phenomena is analyzed by considering the various constituent parts of the simulation hierarchy including the mathematical model of the physics, the numerical model, the computational model (including the mesh), and most importantly the human in the loop. The interactions among these elements are illustrated through examples. The use of Realizability as a goal in obtaining accurate, robust and efficient simulation methods is explained.

1. INTRODUCTION

CFD has become a key contributor in design and virtual prototyping of everything involving fluids. From a broad perspective, CFD is used today in a variety of ways, from supplementing experiments and testing of systems to certification of the performance, safety, and reliability of high-consequence systems.

Assessing the ability and accuracy of a CFD solver can only be achieved through validation and verification efforts. The semantics and definitions for verification and validation are still the subject of discussion throughout organizations such as AIAA and ASME through various publications. Descriptions of verification and validation are given in Table [1]:

Terminology	Definition	Meaning
Verification	"The process of determining that a computational model accurately represents the underlying mathematical model and its solution"	The mathematical model and the solution algorithm are working correctly, and lies within the realm of ***mathematics***
Validation	"The process of determining the degree to which a model is accurate representation of the real world from the perspective of the intended uses of the model"	The discrete solution of the mathematical model is accurate and lies within the realm of ***physics***

Table 1: V&V definitions

The main focus here is to describe a useful integrated and hierarchical way to dissect the practice of computational fluid dynamics (CFD) with the goal of increasing its accuracy, hence effectiveness.

2. SIMULATION HIERARCHY

For our purposes, [2] we define physics as what happens in nature. Simulations of physics are an artificial attempt to mimic that physics effectively enough that it appears as the real thing, with certain practical benefits to be derived based on the ability to simulate. "High fidelity" simulations mimic the physics to a greater degree of match with the real physics than "lower fidelity" simulations. One can think of computational simulation of physics as comprising the elements described in what follows.

The goal is to effectively represent the real physics, where "real" physics is simply a label for what occurs or would occur naturally. In computational simulations, the goal is to define a particular problem that occurs in nature and simulate it using computers. Fluid dynamic problems involve consideration of a volume of space over which we would like to observe the physical phenomena. We may also be interested only in a particular span of time. This extent of space and time is the physical domain of interest. There is then a corresponding computational simulation extent of space and time that represents a continuum, often finite, which may be referred to as the computational domain.

As seen in Figure 1, humans build high fidelity simulations using certain building blocks starting with the mathematical model of the physics. The math model is simply a representation of the natural phenomena that are capable of being manipulated by mathematical analysis. The math model, or the collection of math models representing the physics, is by itself not the solution we are seeking, but the beginning of the means to obtain that solution.

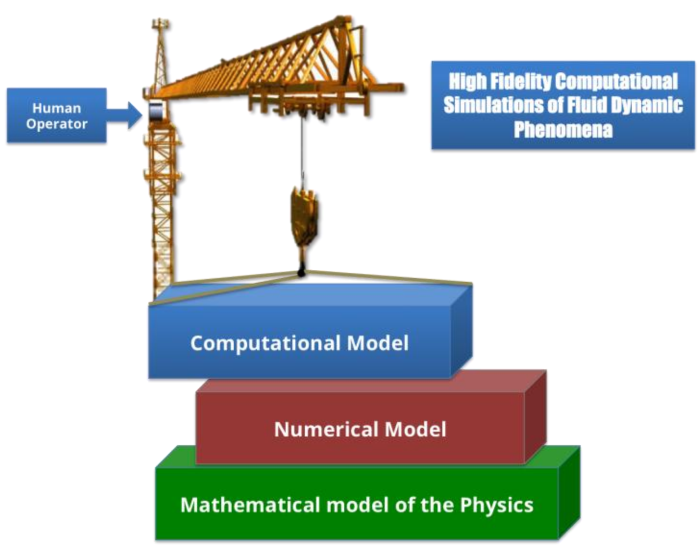

Figure 1: Building blocks of high fidelity CFD

We then create a numerical model or representation of the mathematical model. While the math model is an approximate representation of the real physics, the numerical model is an approximation to the math model. If the math model is once removed from the real physics, the numerical model is then twice removed. The numerical model or method or approach is still not the digital solution we seek. It is still just a means towards that solution.

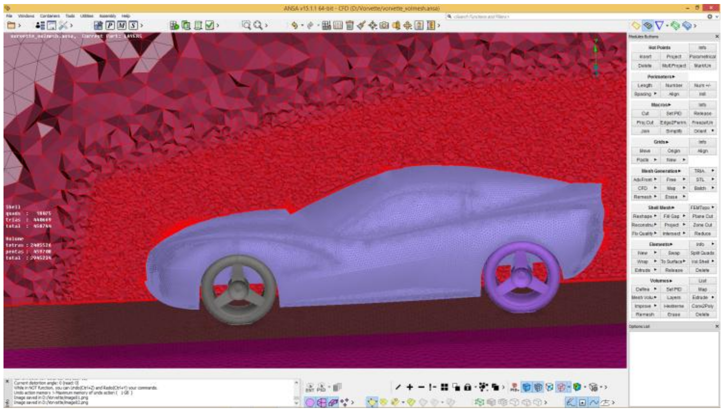

Figure 2: Mesh generation

In computational fluid dynamics and similar fields, the finite continuum is "discretized". One then considers specific discrete points in space and time. In general, one considers a net formed by connecting these points in a certain manner. In this way, the continuum volume is broken up into a finite collection of discrete sub- volumes, each sub-volume made up of relatively simple shapes such as hexahedra, tetrahedra or polyhedra in three spatial dimensions (See Figure 2.) A corresponding discretization of the time span is developed, often as discrete time levels at which the solution is sought. This discretized space and time domain is the computational domain. The mathematical model, in the form of the corresponding numerical method, is applied to this discrete computational domain. This results in a large to very large to extremely large collection of algebraic equations that must then be solved using appropriate techniques on the digital computer.

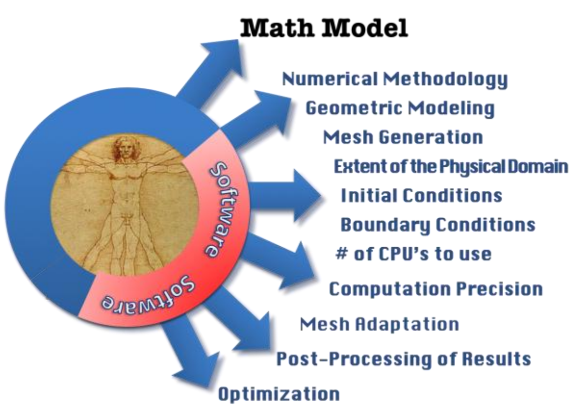

Figure 3: The human factor

Through all this, human beings are very much involved, making decisions at every level of this hierarchy. In order to achieve an effective result, one must carefully consider the human in the loop and not just the technical aspects of the mathematical, numerical and computational modeling. Humans (developers, users, support staff, researchers, engineers, educators, and more) play a critical role in making decisions about the elements of the simulation hierarchy (see Figure 3.) They help decide what types of math models are selected for a particular purpose and they help develop better (or worse) models themselves. They help develop and/or select the numerical methodology to be applied to the math models. They help construct and deploy the computational meshes. Humans develop computational mesh generation tools. They decide on the number and type of mesh cells, the near-wall spacing, etc.

They may develop computer programs, construction tools and diagnostic tools to help with all this, but even in the so-called “automatic mesh adaptation” techniques it is the human that has decided what should be used to guide the adaptation. Humans decide the precision of the computations to be used, the number of CPUs to use in parallel and the amount of computational resources that should be made available to an individual user or a group of users within an organization. Humans decide the extent of the physical domain, the computational domain and the initial and boundary conditions to apply. It is, therefore, very important to take into consideration the human in the loop in order to obtain maximum effectiveness of the total simulation process. In fact, one of the declared purposes of this paper is to increase awareness of the human impact. Another purpose is to channel that awareness by allowing the human in the loop to acquire better knowledge of the process and therefore make better decisions.

3. PROBLEM DEFINITION AND MODELING SELECTIONS

Consider a typical aerodynamic application that could be part of an aerospace or automotive simulation.

3.1. PROBLEM DEFINITION

The practitioner would define the geometry and the physical conditions of the problem. For aerospace applications, this could be as simple as choosing the altitude and Mach number. For turbulent flows, there is a need to define the turbulence environment. Typically, this would be defined in terms of turbulence intensity and a length-scale. These problem definition parameters are strongly related to the physics as nature sees it, still quantified using math model definitions (Mach number, turbulence intensity, etc.). The practitioner must also know/choose if the flow is unsteady or steady or essentially steady and what type of corresponding simulation to choose. The problem definition is woefully incomplete, if there is no definition of what type of information must be gleaned from the simulations. For example, if an accurate knowledge of lift and drag is required at various angles of attack and yaw conditions, such a purpose is best known ahead of time. The choice of math model, numerical model and computational model could all depend on the specific type of information desired. The turbulence model used for attached or mostly attached flow may be different from the model which is best suited for massive separation or unsteady flow or vortex breakdown. It is becoming obvious then, that all elements of the simulation hierarchy are interrelated. Another significant issue is whether we really know, in depth, the true nature of the flow physics that is associated with a particular problem definition. Sometimes the simulation approach is used to try to gain insight into the nature of the physics, but while it can be very fruitful, great care is needed when probing the perfect with the imperfect or otherwise probing natural processes using a model of those processes.

3.2. MATHEMATICAL MODEL

Most math model choices are generally accepted and uniformly applied. This includes the Sutherland or Power law for viscosity and thermal conductivity, the perfect gas equation of state, etc. Furthermore, let us assume here that a form of the Navier-Stokes equations is appropriate. For turbulent flows, the choice of turbulence models is a primary choice to be made, based on the simulation needs. If a turbulence closure can be chosen just based on its suitability for modeling certain physical phenomena, it will be a very good situation indeed. However, often the practitioner may weigh in the robustness of the model in choosing one. The robustness is strongly tied to both the model itself and its numerical implementation. Depending on what model is chosen, the corresponding variables (k, ε, etc.) will have to be defined. The problem definition choices of Mach number, altitude, turbulence parameters, etc., will have to be converted into the corresponding primitive variables (pressure, temperature and velocity components), k, ε, etc. The practitioner must also choose the initial and boundary conditions that are associated with the math model (or the numerical model, as the case may be). For time- accurate simulations, the initial conditions should closely correspond to what would occur in nature. For steady-state applications, the choice of initial conditions could be for a different purpose, merely to help obtain the steady state faster. The practitioners must also choose whether they will employ the “wall function” approach or “solve to the wall”. This has a strong relationship to the type of mesh that must be generated and used.

3.3. NUMERICAL MODEL

The numerical approach requires the choice of the primary numerical method(s) and all the related parameters. Typically, the practitioner must choose inputs that affect numerical dissipation, accuracy (1st or 2nd order, accuracy of the main equations versus those of the turbulence closure, etc.), relaxation (and under-relaxation) parameters, multigrid control, etc. An important consideration in the choice of method is whether an explicit or an implicit type of approach is to be used. This has a strong bearing on success depending on the nature of the computational model (near-wall spacing, aspect ratio of the mesh cells, etc.).

4. INTERACTIONS AMONG ELEMENTS OF SIMULATION HIERARCHY

We present now a few examples of such interactions. We recommend, however, that the practitioners prepare their own tables and charts of interactions (like drug interactions) that pertain to their own operating environment (e.g. the codes that they use). Some of these interactions are generic and apply to most situations; however, some may only be relevant to certain CFD codes or tools.

Solving to the wall implies that a wall grid spacing of Y+ of 0.1 to 1.0 be used. This is an obvious interaction between choice of a turbulence modeling approach and the computational model (the mesh). The solve-to-the - wall approach can often result in large mesh cell aspect ratios in the boundary layer (> 1000 or even > 10000). To accurately balance all the terms being modeled with such large aspect ratios, one may need to resort to double precision arithmetic (this is also a computational modeling choice). A numerical methodology based on an explicit scheme formulation may have a major struggle in obtaining a numerical solution on such grids or to obtain it efficiently. This is an interaction with the numerical modeling. An implicit relaxation method with multigrid treatment that is well implemented may offer good benefits. A code that seems to work well for "wall function" meshes may not fare so well on "solve –to-the-wall" grids. In some numerical treatments, there is so much error (due to extra-large doses of numerical diffusion) that even a mesh spacing corresponding to a Y+ value of 0.1 will not lead to an accurate prediction. CFD codes with such treatments may need a finer grid for accuracy, further exacerbating the problem of numerical stability and rate of convergence. This simple example already illustrates the complexities of the interactions. The impact of the human decision- making process is also obvious here.

For the next example we consider our nonlinear (cubic) k-ε model [3]. Such a model can be better suited for flows with large streamline curvature and allows for anisotropic effects. This model depends more strongly on velocity gradients than a linear k-ε model, therefore a stronger requirement for higher mesh quality exists when using the cubic closure. The mesh should be sufficiently smooth for the velocity gradients (and not just the velocity itself) to be computable with a reasonable level of accuracy and smoothness. If it is not possible to construct a mesh of the desired quality (because of deficiencies in the available mesh generation tools), then, from a practical point of view, a better numerical solution may be possible with a simpler turbulence model on such a relatively lesser quality grid. Here the mesh generation possibilities will have a strong influence on the choice of the math model. We use this example to illustrate how the decision flow is not always one way, from the math model to the numerical model to the computational model, but can also flow the other way. In general, Reynolds-stress models (the cubic k-ε being an algebraically-specified Reynolds-stress closure) are potentially very powerful but to realize their potential, the practitioner must assist by providing the appropriate mesh suitable for the model.

We have frequently observed that mesh, often the one suitable for subsonic flow, is used, very incorrectly, for a very large range of Mach numbers. Not only is it important to consider the outer extent of the computational domain, but also the grid spacing requirements in the boundary layer, as they can be vastly different and thus must be considered in detail.

As a final topic in this section, we consider the unfortunate use of numerical dissipation or artificial ceilings and floors (maximum allowable value or minimum allowable value) to mask the bad effects of weaker math models or computational grids or even numerical treatments. For example, CFD codes may limit the eddy viscosity that would arise in a simulation to an artificially low value. Worse, such limits may be built-in and not obvious to the user. Extra-large values of numerical dissipation or reduced order (1st order) treatment are often used to mask numerical oscillations that would otherwise appear or to mask other numerical instabilities. In the opinion of the authors, it is better to treat model deficiencies in each category of the hierarchy by improving the modeling within that category. This paragraph serves then as an introduction to the next topic: principles that can help develop good math, numerical, and computational models.

5. REALIZABILITY RESULTING IN HIGH FIDELITY

Up to this point, we have suggested that a careful consideration of the interactions among the math model, the numerical model and the computational model can lead to benefits. However, it is also very important for the models themselves to be effective. As we saw in the last paragraph of the previous section, if we begin with bad models, more bad treatments (e.g. numerical diffusion) are required to compensate for undesirable side effects. The infamous GIGO concept (Garbage In, Garbage Out) refers to the fact that computers and software can produce unintended, even nonsensical, output when the input is inconsistent. So, the question we have to ask ourselves is: how can one develop good math models and, independently, good numerical methods? When these are used together with good computational models, quality results can be achieved. Formal (mathematical) order of accuracy is sometimes less important than other physical constraints of the problem that limit the range of the solution. In complex non-linear systems one must, therefore, ensure known physical attributes are satisfied by the solution. This process is referred to as enforcing Realizability.

Here are some examples of Realizability: negative pressures and temperatures should not arise in modeling; negative eddy diffusivities must be avoided. The Schwartz or higher-moment inequalities must be obeyed. Unbounded stress components should not be present. Singularities from vanishing scale parameters should be carefully treated. These constraints are not implied by classical numerical analysis. However, violation of any of these Realizability constraints can lead to failure.

There are two approaches to ensuring such Realizability, one good and one bad. In the good approach, the modeling is done in such a manner so as to avoid non-Realizable behavior. In the bad approach, the non-Realizable behavior will be present in modeling but any resulting unacceptable values will be clipped to be within the desired limits or excessive numerical dissipation will be applied as a “salve” to salvage the situation. Obviously the former approach is more desirable.

We have tried to be true to these principles in our own efforts. In building the turbulence models, for example, we ensure that all normal Reynolds stresses are positive, enforce the Schwartz inequality (Reynolds shear stresses squared cannot be larger than the product of the corresponding normal stresses) and other constraints (time-scale and velocity-scale Realizability). Turbulence models embodying such principles will have less ad-hoc terms, will misbehave less, will not need strange after-the-fact numerical fixes and, most importantly, will yield results that are much closer to physical reality, and hence higher fidelity.

At the numerical level, we have non-oscillatory schemes, which avoid spurious numerical oscillations. TVD and ENO (Essentially Non-Oscillatory) schemes, which the first author helped develop, are examples of such schemes. Early papers on TVD methods referred to themselves as “high resolution” schemes, implying second-order accuracy (except at maxima and minima and shock waves) but most importantly, these schemes avoided numerical oscillations and therefore could capture shock waves with greater fidelity. They also manifested a peculiar property: their nonlinear dissipation reduced to zero at stationary shocks leading to zero thickness or one-cell width shocks. Hence the term “high resolution” was used to classify them.

Also at the numerical level, we have managed to capture the multidimensional nature of real gradients using a multidimensional interpolation scheme. We use an approximate Riemann solver that preserves positivity (does not, by itself, produce negative pressures or temperatures) and satisfies entropy principle. We have found ways to avoid spurious oscillations in the multidimensional interpolation. We have implemented turbulence models in a manner that makes them robust: first through embodying Realizability principles in the model, and then numerically by avoiding explicit fragments. We have found ways to ensure positivity in modeling the terms that represent physical diffusion by employing carefully designed discretization in the vicinity of highly skewed cells.

6. CONCLUSIONS

In summary, the hierarchical elements considered are

- Physics of the problem at hand
- Mathematical model of the physics
- Numerical model of the math model
- Computational model of the numerical model
- Human in the loop
- Resulting computational simulation and its relationship (fidelity of representation) to the physics being modeled and simulated

All this is rather obvious. However, there is significant benefit in making the effort to consciously consider this hierarchy and the interrelationships among the constituent elements. We have highlighted in this paper, benefits in the following areas:

- Development of high fidelity simulation techniques and corresponding high fidelity computational solutions
- A framework to learn and adhere to “best practice” techniques (processes) and increase productivity for the organization that is using CFD to achieve its design or analysis goals
- A framework or environment for users of CFD tools to learn and improve their own skills and become better practitioners
- A framework that helps support staff to better diagnose problems that arise in the use of CFD tools and more efficiently and effective help users.

A hierarchical perspective of various constituent elements of the computational simulation process has been presented. The elements and their mutual interactions have been discussed through examples. A philosophical framework for the development of good mathematical and numerical models has been outlined. These ideas are not just concepts, but have been embodied and tested thoroughly in the CFD++ software suite. The ideas have helped develop CFD simulation software that is robust, accurate and efficient even on massive and highly clustered meshes.

7. REFERENCES

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