Comments on the Third Lisbon Workshop on Uncertainty Assessment in CFD

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Introduction

The Third Lisbon Workshop on CFD Uncertainty Analysis is now over. Just like after the Second Workshop held in 2006, I am back in my office pondering this event and its significance. Again, I am impressed by the format which left ample time for discussions. This was one important ingredient making this event the success it has turned out to be. It allowed us to share our successful experiences as well as our failures to maximize both our learning and the benefits we drew from this exercise. For my part I learned a lot. Thank you to all those who made presentations, asked questions, and made comments.

General observations on code and solution verification

The level of consistency between predictions using the same turbulence model has increased since 2006, an indication that we, as a community, have improved our ability and capacity for quality work. The degree of grid convergence for the manufactured solution is quite good and exhibits consistency across codes for U_x and C_p. Code verification seems to have come of age, at least for this group!

The level of consistency across codes for the solution verification of the backward facing step turbulent flow also appears good for U_x when enough grid points are used and numerical uncertainty estimates are small. I find it very comforting that the least-squares approach of Luís and Martin incorporating the data range can be applied to grids that are not in the asymptotic range of the discretization scheme. Albeit, with the caveat that in such cases on must accept the very large uncertainty intervals that are predicted. I am encouraged by the fact that it appears to be a self diagnosing process: uncertainty intervals can be estimated and when they appear ***too large***, they serve as a warning sign that our simulations and grids are likely outside of the asymptotic range.

On uncertainty estimators

I was also impressed initially by the variety of new uncertainty estimators presented. New ideas and techniques are exciting to discover, study, and use. However, their proliferation makes the rigorous testing and thorough comparison of their performance, a daunting, if not impossible task. Such a situation would obviously be detrimental to numerical uncertainty assessment. And counter productive for the development of procedures that may have a reasonable chance of being accepted at large by the CFD community. Let alone of making their way into *Standards*. The question then is: on which techniques should we edge our bets and focus our efforts to test uncertainty estimators on a sufficiently large and diverse set of test problems.

Adaptive Remeshing: is the fruit as ripe as it appears?

Participants have commented or observed that Adaptive Remeshing appears to offer and to deliver the degree of grid refinement needed to reach the asymptotic range of RANS solvers. Some of my colleagues went as far as to say it was the way to do it. It is a fact that few if any other technique can deliver the very high and extremely localized refinement ratios observed in adaptive remeshing. In Lisbon, I quoted that the ratio of the length of the shortest edge of the coarse mesh to that of the fine grid was approximately 5,400. This is equivalent to an area ratio of 23×10^6 for this 2-D problem! Needless to say that robust numerics are a must to handle such extreme grids. Scaling to 3-D yields a volume ratio of 11×10^9; a scary thought...

Adaptive grid refinement by local subdivision of elements, also known as h-refinement, (element edges split into 2, triangles into 4 and tetrahedra into 8) could achieve similar ratios. However the 12 to 13 levels or generation of refinement (2^{12} = 4,096 and 2^{13} = 8,192) would generate much larger grids because the refinement is more gradual: two edges will differ by factor of 2 on average. H-refinement amounts to localized grid doubling. We all know how expensive global grid doubling is. While the local variant is more effective than its global counterpart, it still generates huge grids. Elements with an error estimate larger than the target value are flagged for refinement and its edges are split into two new edges half the size of the parent edge. This sets the degree of refinement to 2 per level of h-refinement. Furthermore, splitting a tetrahedron into 8 sub tetrahedra yields 4 elements geometrically similar to their parent (the 4 associated to the vertices of the parent tetrahedra). The remaining octahedron can be split into 4 sub-elements. However, they are not similar to their parent, they will be somewhat flatter. Further h-refinement of such flatter tetrahedra will eventually lead to sliver or degenerate elements that are detrimental to most solvers. Some corrective steps must be implemented to remove sliver elements or improve their shape.

Adaptive remeshing is free of such constraints because the values of the local error estimate, the target error and the convergence rate are used to estimate the local element size. Hence, adaptive remeshing can vary the local refinement ratio in a continuous manner throughout the domain to either coarsen the grid or refine it by an appropriate value determined by the error analysis and the transition operator (rule to decide the local mesh size). The net result is that adaptive remeshing will exhibit mesh size variation that are much More rapid yet smoother than those obtained by h-refinement. There is a price to pay for this added advantage. Adaptive remeshing is more demanding on the grid generator. The algorithm for mesh generation must be very robust to ensure that a valid mesh is obtained for a given grid density distribution. H-remeshing is relatively simpler to implement. If the current mesh is a valid one, then the grid obtained by h-refinement will also be valid. Remeshing does not offer such guarantees. I am not sure that current unstructured 3-D mesh generators and solvers are robust enough yet.

Also, we used isotropic grids (nearly equilateral triangles). I believe this will not be feasible in 3-D. Stretched meshes will be required. Their automatic generation is a non trivial task and doing it adaptively will require more research to come up with a technique to relate error estimates to not only local grid size but also element stretching and orientation. Such a technique must be capable of handling multiple solution fields which may present conflicting stretching requirements along two distinct directions for two separate flow variables. While such adaptive techniques have been demonstrated for inviscid flows, there is much work to be done for viscous flows, and incompressible flows.

Thus, while adaptive remeshing appears sufficiently robust and mature for V&V in 2 dimensions, it appears that its 3-D counterpart is not yet ready for industrial applications. We should expect that the more traditional block structured grids are here to stay for some time (even if Luís himself has announced his intention to go unstructured! I am sure he will come up with more ways to surprise us). Block structured grids can serve as an initial grid of hexahedra that could be converted into a mesh of tetrahedra which would then be h-refined. Performing 3 to 5 cycles of h-refinement might be sufficient for V\&V and RANS simulations provided that initial coarse mesh is good one. I will defer to my colleagues in naval hydrodynamics to tell us whether this is feasible. Another idea could be to use single grid error estimators for the block structured meshes to provide guidance and some feedback to create an improved block structured grid and generalize the least-squares technique to use such data to produce uncertainty intervals

Validation

I was very impressed by the two approaches to Validation. The first one consists in plotting predictions and experimental data each with it uncertainty intervals or bands. To me this appears as an important step forward for CFD. The reporting of CFD results is now one step closer to that of experimental methods which have a long history of reporting data with uncertainty intervals along with the uncertainty analysis. The second approach to validation was somewhat of a revelation and seems to offer a great deal of potential if we use it properly. Plotting the Validation uncertainty U_{val} and the Validation comparison error E provides significant insight as to whether (and where in the domain) the modeling error can be reduced by improving the turbulence model, $|E| >> U_{val}$, and where improvements are more problematic because the modeling error is of the order of or is smaller than the Validation uncertainty U_{val}.

Input data uncertainties and weak models

The validation procedure used for the workshop is a simplified version of the V&V 20 Standard, soon to be released. It assumes that there are no uncertainties in the input data to the CFD code. In other words, it assumes that the fluid properties, the boundary conditions, the geometry of the domain, and the turbulence closure coefficients are all known exactly. Of course it seldom is the case, as was revealed at the workshop: a systematic discrepancy in the velocity profile near the top wall was observed across all codes and turbulence models that were tested. This is an indication that the data used for the inflow velocity profile carried an uncertainty, especially near the top wall, that was not accounted for.

Estimating the impact of such uncertainties on the flow predictions implies performing an uncertainty analysis to cascade the input uncertainties through the CFD code to obtain an estimate of the uncertainty on the flow response. There was not enough time at the workshop to discuss this issue. The uncertainty analysis is very much the same as that used in experimental work. Sensitivities of the predictions must be evaluated, that is the partial derivatives of the dependent variables, with respect to the parameters of interest. For example, $\frac{\partial u}{\partial U_0}$, $\frac{\partial p}{\partial k_0}$, and $\frac{\partial k}{\partial C_\mu}$ are the sensitivities of the streamwise velocity component with respect to the inflow mean velocity, of the pressure with respect to the level of turbulence kinetic energy (TKE) at the inflow plane, and the sensitivity of the TKE with respect to C_μ one of the closure coefficient in the k-ε model. They represent, to first order, how the flows would adjust to a unit perturbation in the parameter of interest. Just like the flow variables, the flow sensitivities are computed over the whole domain. The uncertainty analysis proceed in the same manner as the one describe by Coleman and Steele, the only difference being that in standard engineering application uncertainties and sensitivities are real number while here they are functions of x and y.

These derivatives can be computed by one of several techniques: finite difference quotient of two flow solutions at slightly different values of the parameter, the complex step method, the discrete sensitivity approach or by the continuous sensitivity equation method. Here too, verification will play an important role in ensuring good numerical accuracy. The important issues are:

- to have access to these derivatives to perform the uncertainty cascade
- to have some idea of their numerical accuracy

It is also important to understand that this approach to uncertainty assessment of weak models is feasible now, and likely to be another important step forward for CFD.

Conclusion

The Third Workshop was a success on all counts. We made real and tangible progress in our understanding and use of the Method of Manufactured Solution for code Verification, in simulation Verification (we can reach the asymptotic range for the RANS equations), the combination of the leat-squares Richardson extrapolation (variable order) and disarrange provide uncertainty both in the asymptotic range and outside. However, in the latter case the uncertainty estimates may seem uncomfortably large.

The success of events like this workshop depend heavily and almost exclusively on the commitment and will power of their organizers. We owe many thanks to Luís Eça and Martin Hoekstra for the organization and preparation of the three workshops, for the

open discussion, for their interesting conclusions, and their unique interventions. It is my belie that we would not have experienced the high level of success that we have, had it not been for the warm hospitality and friendship of our hosts who took it upon themselves to share with us a bit of their Portugal, its people, its delicious food, and wonderful Port wines. I have had a wonderful time in *Lisboa* and I made many new friends. To all of participants, I say thank you.