Overview of "Workshop on CFD Uncertainty Analysis"

Patrick J. Roache

Executive Summary

The subject Workshop aimed at evaluation of CFD Uncertainty Estimators by comparing results of six groups on two fluid dynamics problems involving separated turbulent flows. Various CFD methods were represented, and calculations were done on smooth grids as well a deliberately poor grids in order to burden the Uncertainty Estimators. Even though local grid convergence was often oscillatory, the overall consensus evaluation was generally favorable for the Grid Convergence Index (GCI) and the Least Squares version of it, as well as a monogrid Error Transport Equation (ETE) method. Some residual doubts remain on the inter-group comparisons because of conceptual modeling differences and the possibility of undetected coding errors. These could be eliminated by the use of a realistic exact analytical solution produced by the Method of Manufactured Solutions, and the consensus favored this approach for a second Workshop on this theme. The consensus opinion was also clear that the Lisbon Workshop was successful.

Objectives

A "Workshop on CFD Uncertainty Analysis" was held 21-22 October 2004 at the Instituto Superior Técnico in Lisbon, Portugal, sponsored by IST and MARIN of the Netherlands. There were 35-50 persons in attendance, including observers. The groups presenting calculations were from Italy, Germany, USA, France, Bulgaria, Japan, and Portugal/Netherlands. I was honored to present the keynote address.

To evaluate Uncertainty Estimators, two problems from the ERCOFTAC Classic Database were used: C-18 Flow over a Hill at Rn = 60000, and C-30 Flow over a Backward Facing Step at Rn = 50000. Both exhibit turbulent separated flow. Three turbulence models were used by various groups: the one-equation models of Spalart-Allmaras and of Menter, and a version of k-epsilon (Chang Hsieh and Chen). The CFD codes used represented both in-house and commercial codes and included various FVM and FDM, strong or weak conservation from, and various flux limiters and artificial compressibility methods, with formal orders of accuracy varying from p = 1, hybrid, 2, and 4. Most of the calculations were performed with very tight iterative convergence criteria, and grid convergence was evaluated in several error norms.

The Workshop organizers had distributed to participants sets of single-block, geometrically similar grids, thus eliminating non-similarity as a cause of noise in grid convergence tests. This also encouraged participation by eliminating the grid generation work, including the attention paid to turbulent sublayer resolution. For the Hill, two grid sets of 11 grids each were provided; participants were free to use as many or as few as they chose. The first family was nearly orthogonal, while the second was deliberately designed to burden the Uncertainty Estimators by departing significantly from orthogonality (maximum deviation angle 40.5°). For the Backstep, three grid sets of 7 grids each were used (maximum deviation angle as high as 63°). The grids were acknowledged to be of good quality for the hill and poor quality for the backstep; this was deliberate, in order to burden the Uncertainty Estimation methods. A strong discontinuity in the grid first derivative was propagated from both the backstep corners (external and re-entrant). Further burden was provided in the Backstep Problem by the third grid set which deliberately did not place any grid nodes coincident with the backstep corners; this added significant discretization error for the FVM.

The Workshop Organizers wisely did not include any ERCOFTAC data on the experimental values, emphasizing that the topic of the Workshop was Verification of Calculations, not Validation. This distinction was well recognized and appreciated by all the participants.

Methodology and Goals of the Comparisons

Three Uncertainty Estimation methods were used by various participants: the 3-grid Grid Convergence Index (GCI) with Factor of Safety Fs = 1.25, the Eça-Hoekstra Least-Squares version of GCI also with Fs = 1.25, and an Error Transport Equation Method (with implicit Fs = 1, i.e. an error estimator).

Participants agreed that the evaluation of the 95 % Uncertainty Estimators U95 or Error Bands should be based on the following performance criteria. On any one mathematical problem, if the exact or benchmark solution is known a priori (not the case here) or can be well-bounded by the finest grid solution, then the Uncertainty Estimators for the coarser grid sequences can be simply evaluated; the benchmark solution should lie within the error bands over the fine-grid solution of any grid sequence in roughly 95% of the cases. Alternately, without considering possible vaguaries of evaluating a benchmark, the Uncertainty Estimators can be evaluated for internal consistency; on any one mathematical problem, all the Uncertainty Estimates from various grid sequences should roughly overlap.

For example, Participant “A” might calculate solutions with a hybrid-order strongly conservative FVM on a 4-grid sequence selected from the coarse end of the grid set provided. To estimate the U95 for the solution S(A) on the finest of these 4 grids, Participant “A” might use the Least-Squares GCI; call this U95(A). Another Participant “B” might calculate solutions using a 4th order weakly conservative FDM on a 3-grid sequence from the fine end of the grid set provided. To estimate the U95(B) for the solution S(B) on the finest of these 3 grids, Participant “B” might use the standard 3-grid GCI. It is to be expected that solution S(B) will be more accurate than S(A), and that U95(B) < U95(A). But when these error bars are added to the respective flow calculation from each solution, the results should overlap, i.e. S(A)±U95(A) should overlap S(B)±U95(B) in roughly 95% of the cases.

This of course assumes that the same mathematical problem is being calculated by both participants. There is no reason to expect that the solution ± error bar for the Spalart-Allmaras turbulence model applied to the backstep will overlap that for the Menter model. (Large disparity would indicate a Validation issue for at least one of the turbulence models, but our U95’s may be smaller than the modeling discrepancy. In fact, this is the necessary condition for a meaningful distinction of the models in Validation.)

Results

In fact, this goal of overlap of Uncertainty Estimates was essentially met by the Workshop contributions, but not always. Opinions were actively solicited from the participants, both calculators and observers. The clear consensus was that the results were gratifyingly consistent and provided a favorable evaluation for all three approaches to Uncertainty Estimation. This was true even though some of the apparent superconvergence results (e.g. observed $p = 2.5$ for a formal $p = 2$ method) were used (rather than the more conservative recommended approach of limiting p to formal order in the GCI formula), and in spite of the fact that many of the grid convergence tests displayed oscillatory convergence in local values. As expected, functional values like base pressure or integrated friction behaved better than did local values.

It was noted and agreed that oscillatory convergence does not indicate that the CFD solutions are necessarily inaccurate, even though it may make Uncertainty Estimation more problematical. In any case, oscillatory convergence is a property of the CFD solutions on the grid sequence, not of the Uncertainty Estimation method, and participants were urged to not "shoot the messenger."

However, some disparities remain, and unfortunately it cannot be ascertained whether or not the shortcoming is essentially the behavior of the Uncertainty Estimators. In spite of the best efforts by the Workshop organizers and participants, the mathematical definition of the problems in fact varied. One source was differences in boundary conditions: not merely the numerical implementation (which involve only ordered errors and therefore are estimatable in a grid convergence test) but in the continuum definitions, particularly at inflow and outflow. The IST/MARIN group suggested that these conditions could contribute to the remaining disparity. (Specified outflow velocity values degrade the answer, whereas specified gradients degrade the grid convergence behavior.) Also, it is widely recognized that different codes using nominally the same turbulence model can differ in detailed implementation enough that the continuum answers differ. (Although the differences might be insignificant compared to Validation tolerances, they might be large enough to pollute these evaluations of Uncertainty Estimators, which necessarily involve greater than typical grid resolution.) Further, there remained lingering doubts about the possible role of coding errors, i.e. Verification of Codes.

Recommendations for Future Workshops

Both of these difficulties can be avoided in the next Workshop on this theme, if one is held. (One possibility is a mini-symposium in connection with the Eccomas CFD Conference in 2006.) A realistic exact analytical solution can be generated using the Method of Manufactured Solutions (MMS). This can be done by the next Workshop organizers, and the solution provided to the participants. Some solutions for candidate problems of interest already exist (e.g., a turbulent impinging jet) and others could be developed for specific physical problems and turbulence models. With an exact solution available, participants could remove any doubts about coding errors and the effect of computational boundary conditions. It is only necessary that the codes used be capable of treating source terms (which involve no derivatives) and (possibly) non-homogenous boundary values. Fore example, outflow gradients which are usually modeled as zero could be set to their exact values. Alternately, the usual conditions can be used (e.g. the "natural" FEM condition) and the effect of this continuum conceptual model on the answer can be evaluated independent of the assessment of the Uncertainty Estimator. Once again, there was strong consensus that any further Workshop with this theme should utilize this approach.

It was also agreed that any future Workshop should specifically invite participation by groups using unstructured grid [or grid-free] CFD solutions. Known applications of the GCI to unstructured grids using a crude "effective grid refinement ratio" have been ad hoc and highly limited. A more extensive evaluation using a systematic approach and an exact solution would be welcome. Also, experience with application of the Fs > 1 to an Error Transport Equation approach would be welcome, although this is easily performed as a post processing step. (If the ETE approach is consistent, as it appears to be, then the error estimate obtained by ETE should be consistent with that obtained by Richardson Extrapolation, and the same value of Fs used in the GCI should apply to the ETE.)

It was generally agreed that more extensive problem sets and more difficult problems should be addressed at some time in the future, but that the next Workshop should still be limited to one or two simple problems. Comparisons are difficult, even with simple problems. The limitation to simple problems will both encourage participation, and will keep out extraneous factors that could confuse a definitive and convincing evaluation of Uncertainty Estimators from a broadly based segment of CFD practitioners.

The now-standard methods apparently work well enough even for oscillatory convergence. Although the theoretical basis for the Richardson Extrapolation and GCI is then undermined, the empirical use of a Factor of Safety and/or the Least Squares evaluation of observed order usually proved successful. There was some interest in attempting to develop new methods designed specifically for oscillatory cases.

Final Remark

Regardless of whether or not a future Workshop on this theme is held, the October 2004 Lisbon Workshop will be remembered as one of admirable participation. Throughout there was a sense of honesty, intellectual pursuit, and international cooperation. Presentations and discussions were both candid and respectful. The organizers and participants (both calculators and observers, who also participated in the discussions) are to be congratulated for this successful and exemplary exercise.