Incremental Costs and Benefits of Calculation Verification

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While CFD practitioners may shrink from the idea of performing multiple-grid studies, the following observations on the incremental costs and benefits of thorough Calculation Verification are relevant.

First, unless your code contains some single-grid error indicator [1], at least two grids are absolutely necessary in order to obtain any *quantified* estimate of numerical uncertainty. Even if the code uses something like the Zhu-Zienkiewicz estimators, which is highly recommended [1], these do not provide error bands for the quantities of engineering interest, and by themselves (in a single grid calculation) can provide no indication that the actual rate of convergence is adequate.

Thus, two grids are a minimum for *quantification* of error bands. But these two grids need not represent a doubling in each direction; in fact, there are advantages besides economy to using less than integer coarsening/refining [1], e.g. ~10% coarsening. For example, we may want to verify the calculations on a grid of 100 cells in a direction, and obtain our error bars for this grid solution by obtaining another solution with 90 cells, Note this is cheaper than the original solution, so the computer cost is less than doubled. More importantly, the human cost is far from doubled. The incremental human cost to run the second grid solution should be amortized over the problem set-up time, including decisions on type of boundary conditions, etc.

Given the fact that two grids are a minimum, and that integer-grid coarsening is not required, consider the incremental costs and benefits of obtaining more grid solutions. An obvious upper bound for the incremental work (computer and human) to obtain the third grid solution is 50% (3 solutions instead of 2) but this is not at all a tight upper bound. If the third grid uses 80 cells, and if the problem is 3-D time dependent, and if optimal efficient solvers are used, and if the time step is correctly scaled along with the grid size, then the computation time varies [1] as Δ^4. If the base (100-cell) grid cost is 1, then the 90-cell and 80-cell solutions cost 0.66 and 0.41. The incremental computer cost for the third grid is 0.41/1.66 = 0.25. (The incremental cost is much less than 25% if non-optimal solvers are used. For typical point-iterative elliptic solvers, which dominate the costs, the variation is Δ^5 or more.) The incremental human cost is probably less than this 25%.

For this roughly 25% incremental cost, what is the incremental benefit? The gain in credibility and confidence is very significant indeed. Convergence rate is now *verified*, rather than assumed. The GCI factor of safety can be confidently reduced from 3 to 1.25, so that a previously reported error band of (say) 12% can be reduced to a more optimistic 5%. The confidence of all readers (or customers, regulators, stake holders, etc.) is justifiably increased as *evidence* is provided to demonstrate that the modelers are serious about assessing accuracy.

Further work produces yet higher benefit-to-cost ratios, provided that the coarsest grids used are still in a reasonable range. With least-squares determination of observed order of convergence p, or perhaps other intuitive approaches to use multiple grid triplets (e.g. averaging p from each of the four triplets in a four-grid sequence, or weighting the p from the finest grid triplet) reader confidence turns to admiration; if the results are demonstrably well-behaved (e.g. monotonic and in reasonable agreement with theoretical p) then numerical accuracy is no longer a divisive issue.

Further, it is important to bear in mind that these verifications need not be performed on every calculation in a large study if many of the problems are "nearby" to one another, in the sense of parameter ranges and dominant physics. This will be the situation when large numbers of parametric runs are performed on nearly the same geometry, e.g. in design studies in which the various geometries are highly derivative of one another.

In summary, consideration of the incremental costs and benefits of thorough Calculation Verification makes a very good professional and economic case for increasing thoroughness in Verification of Calculations using the methodologies described herein.

[1] - Roache P.J. – "Verification and Validation in Computational Science and Engineering" - Hermosa Publishers, 1998.