Need for Control of Numerical Accuracy

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The need for the control of numerical accuracy in computational fluid dynamics (CFD) code solutions is reviewed in the light of current journal practice and experience with implementation of an editorial policy on the same subject published by the *Journal of Fluids Engineering*. Various actual objections to that policy are listed and responses are given. The general successes and particular difficulties experienced in the implementation of the policy are noted. The broader question of code verification, validation, and certification is considered. It is suggested that professional societies such as the AIAA and American Society of Mechanical Engineers may ultimately become involved in the task of certification of commercially available CFD codes.

I. Introduction

THIS paper, on the general philosophy and need for numerical accuracy control in computational fluid dynamics (CFD) codes, is based on experience with the implementation of an editorial policy statement by the American Society of Mechanical Engineers (ASME), published in the *Journal of Fluids Engineering* (*JFE*).[1] The policy statement was conceived following the creation of the position of Associate Editor for Numerical Methods in the *JFE,* which formally recognized the special needs of this discipline. The ASME policy and supporting statements are reproduced in the Appendix. The rationale and needs for the policy statement are explained in the announcement. The *JFE* had previously published and had many years of experience with a similar requirement for uncertainty analysis in experimental papers. Following our early experience with this new policy, a similar policy was also adopted by the ASME's *Journal of Heat Transfer*. The general subject of control of numerical accuracy has become something of a "hot topic," with special reference to the National Aero-Space Plane, a session at the AIAA 1989 Thermophysics Conference, ASME sessions at the 1988 and 1989 Winter Annual Meetings, and by the Texas Institute for Computational Mechanics workshop on the slightly broader topic of reliability in computational mechanics in October 1989.

II. Resistance and Objections

Although Roache et al.[1] thought that the policy statement and the editorial requirement were quite mild, it was not universally welcomed. Objections were offered by some of the other editorial board members and by other members of the professional community from whom I solicited comments in the months following the publication of the statement. Some of these objections, all of which are actual (i.e., not straw-man objections), are listed below, together with my responses.

Objection 1

It is too expensive of computer time to do mesh doubling calculations in order to ascertain grid convergence.

There are, of course, other ways to ascertain grid convergence than the straightforward method of grid doubling. In fact, this is probably the most reliable method available, but there are other approaches, as briefly touched upon in the original policy statement. If the cost of computer resources is not a problem to the researcher, this is certainly the easiest approach to take. However, if computer resources are a problem, there are other methods that are not intensive users of computer time. It seems that the greater objection for doing grid convergence studies is the fact that it requires a bit of conscientious work on the part of researchers.

Also, if it is argued that it is simply too expensive to do any kind of control of numerical accuracy, then I would argue that the author simply cannot be in this CFD business. After all, if you do not have a wind tunnel you cannot do experimental testing. My impression of the situation is actually worse than this. Journal articles in the late 1960s and early 1970s commonly predicted high resolution accuracy runs when the next generation of computers became available. But for the most part they have not been used that way. Generally the tremendous advance of computing power has been used to produce more mediocre papers rather than fewer reliable ones.

Objection 2

Some exception to the policy should be made for expensive calculations, particularly three-dimensional turbulent studies.

I do not think that the overall cost of the computations should be a consideration. It seems clear that the incremental cost of performing a grid convergence test should be normalized by the cost of the base case. In this sense it is cheaper to validate the grid convergence on a three-dimensional problem than on a two-dimensional problem, presuming that the incremental work involves an extra coarse grid computation. This again relates to the first point, which states that it is not necessary to do a grid doubling in order to ascertain some index of numerical accuracy. A grid halving is also appropriate. Of course, the advantage lies in doing a grid doubling test because the error bounds will be sharper.

Objection 3

Turbulence modeling, rather than the numerical solution of the partial differential equations, is the real determinator of accuracy.

My response is, yes and no. Accuracy is a question to be addressed even for laminar flow calculations, wherein the constitutive equations are not in doubt. The discretization error does not disappear just because one uses a turbulence model! Our point in the *JFE* policy statement, and the first criticism which our evaluation committee made at the 1980/81 Stanford meeting on complex turbulence flows,[2] is that one cannot evaluate different turbulence models unless one first satisfies grid convergence. There are yet more considerations

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in the overall accuracy question; including, for example, the attainment of a true steady state in the computations (yet another "convergence"), inner-loop convergence for incompressible flows, equation of state accuracy, low Mach number approximation, geometry representation, accuracy of viscosity and conductivity coefficients, constant Prandtl number assumptions, chemical reaction rates, and so forth. And, of course, coding errors! These all affect accuracy but do not remove or over-ride the requirement for grid convergence testing. I am of the opinion that these modeling questions, including turbulence modeling, should be kept separate from the question of the numerical accuracy of the solution to those mathematical models.

However, there is in fact another special problem with turbulence modeling in that both the fine and coarse grids have to get some points into the viscous sublayer. I do not know any easy way around this or any other problem that generates such a range of significant length scales which must be adequately resolved. However, thorough work can be done. See, for example, Ref. 3.

Objection 4

The policy statement does not go far enough.

This is certainly true. We consider the *JFE* policy statement to be a minimalist statement. The idea is to make it clear that the authors have to address the topic of numerical accuracy control, and to give the editors and the referees the support they need in demanding some effort in this regard. For example, in the policy statement, no mention is made of the control of errors due to far-field boundary conditions. Cheng[4] pointed out two decades ago that this computational modeling error does not improve as the grid is refined. The only way to test for its effect is to move the position of the far-field boundary. Likewise, the simple reporting of, for example, a 5 or 10% difference in some function of the solution between two grids is not really a rigorous indicator that the solution has been obtained to 5 or 10% accuracy. Although claims have been made that the finite-element methodology offers a more rigorous approach to error estimation, I have not been convinced that anything useful and dependable has been produced for nonlinear systems of partial differential equations. (The theoretical work that has been done is interesting to some extent, but it is usually limited to a very simple model equation.) Schonauer[5] has devoted much time and effort to producing accurate error estimators for Navier-Stokes codes. In fact, his goal is not merely to produce accurate solutions but to accurately predict the error bounds on those solutions. I suppose a really tough journal policy or certification policy would require such effort before accepting a solution, but the journal policy that we adopted was much more lax than this. The only intent was to avoid the syndrome of producing a single calculation on a single grid (the all too common "take it or leave it" attitude).

It is important to note here that grid convergence is really only one aspect of numerical accuracy control; it is, however, a necessary component. For example, a statement of results on grid convergence studies really has nothing to do with coding errors (unless an exact solution is known, as will be discussed subsequently).

Mehta[6] is concerned with code validation, verification, and certification. Note that a *code* is certified, but a particular calculation still needs to be examined for the control of numerical accuracy. A wrong code can "converge" and, conversely, a correct (i.e., certified) code can be applied to a particular problem with an inadequate resolution. Therefore the question of grid convergence testing really presumes ahead of time that we have a correct code. The only question then remaining is whether or not the code has been applied with adequate resolution to obtain an accurate answer to the problem at hand.

Common sense and experience certainly indicate that this presumption of code correctness is not always justified. There are now tools available to perform this kind of verification quite convincingly, in my opinion. In Ref. 7, we showed how to verify a FORTRAN code that was produced entirely by a symbolic manipulation code. The idea is to generate a selected analytic solution to a problem by introducing forcing terms and then to monitor the convergence of the CFD code to that solution as the grid size is reduced. This procedure verifies the coding accuracy, the grid transformation equations, and even the order of accuracy of numerical method. In Ref. 7, it was performed only for the Poisson equation in a transformed three-dimensional coordinate system and for the most common elliptic grid generation equations. Shih et al.[8] have applied this concept to the full incompressible Navier-Stokes equations in two-dimensions. I consider this paper to be one of fundamental importance in the area of code verification. It would seem that the principle can readily be extended to compressible and three-dimensional flows using symbolic manipulation programs such as MACSYMA. Turbulence models also appear to be amenable to this approach of accuracy checking—noting of course that we are not talking about the adequacy of the turbulent representation of the real physics but rather the correct coding and the numerical solution of the turbulence model. Shocks, however, seem to be a more difficult topic to approach in this manner.

Note that there is an earlier history of using very simple solutions to verify models, but false indicators of accuracy sometimes have been obtained. The key in such an exercise is to choose a solution with enough structure in it to exercise all of the terms in the equations and all of the leading error terms in the discretization. If, for example, one selects a Couette flow solution, one will be lead to the erroneous conclusion that a first-order accurate method is perfectly adequate even with a coarse-grid resolution. The power of the Shih et al. method[8] is that the particular solution they have constructed behaves like a real fluid dynamics problem with boundary layers and significant solution structure.

Objection 5

First-order methods and hybrid methods are not more difficult to judge for convergence than second-order methods, contrary to the discussion in the policy statement.

I do not understand this objection. It is an elementary behavior of numerical methods that higher order accurate methods, as they approach convergence, do so more quickly. For example, a fourth-order Runge-Kutta method applied to an ordinary differential equation is easier to judge as being converged than is a second-order method. If a paper reports that a successive grid doubling of a solution of a linearized advection-diffusion equation produces only a 5% change in the answers, one could expect with some confidence that the fine grid solution is indeed within 5% of the true solution, if the method used is fourth-order accurate. If the method used is second-order accurate, it is more problematical; if the method used is only first-order accurate, I would be skeptical of the 5% limit on the "accuracy."

Objection 6

Agreement of the calculations with experiment is enough justification for the solution accuracy, without any need for doing systematic grid convergence testing.

This objection is quite attractive at first glance. In practice, it does not seem to work very often because the agreement with the experiment is usually not universal. This is especially obvious (as stated in the original policy statement) with turbulence modeling. Whether or not the turbulence parameters have been "tuned" to a particular problem, we still have a "package deal" of discretization errors and turbulence modeling errors. The discretization errors should be separated from the turbulence modeling errors. If constitutive equations are not an issue, and if the agreement with a very good experiment is complete, I suppose I would have to relent. But I would still maintain that a *better* paper would result if two grids or some other grid convergence testing were used. For one thing, it would give some idea of how difficult the problem is numerically. (For example, perhaps the results presented were on 100×100 and a 30×30 grids might have been sufficient.) Also, such an exercise may help to verify the code, and would also verify the order of convergence of the code. As Blottner[9] demonstrated two decades ago, plausible second-order, boundary-layer approximations in fact do not always behave in a second-order manner, and this rate of convergence can be established by a systematic grid refinement testing.

Objection 7

I do not have any "truncation error" in my solution since I use finite-element methods (FEM).

Sure you do! (Whether or not the Taylor series is used in the *derivation* of a discrete method, it can still be used in an *analysis* of the method.) But it would have been better in the *JFE* policy statement if we had used the more general term of "discretization error." (Also, "truncation error" strictly speaking is not applicable in the presence of discontinuities.) I would also note that the commonly referred to FEM "error evaluation" practice of substituting the basis function and the solution values into the original partial differential equation is perhaps a valid index of discretization error, but it is not absolutely the error evaluation that we ultimately want. That is, this procedure does not tell us the difference between our discrete solution and the exact solution.

Objection 8

It should not be necessary to legislate such a requirement for doing conscientious work.

It should not have been necessary, but it was. The need is indicative of the problem; that is always the case for legislation, rules, formal ethics committees, and so forth. If a 25th-century historian were to read through Albuquerque newspapers from 1989 he would find Sunwest Bank advertising that it has been "Safe, Strong, and Sound for 65 Years." The historian would rightly conclude that the U.S. banking industry in 1989 was in trouble. He would also read a lot about congressional ethics committees and rightly conclude that political ethics were somewhat lacking. And if he read our *JFE* policy statement on the control of numerical accuracy, he would rightly conclude that there was a bit of sloppy work going on. As Professor George Raithby wrote to me after Ref. 1 was published, "The need to legislate that authors check accuracy is sad, but the enforced discipline will benefit the field."

III. Difficulties in Applications

Generally speaking, the response from the reviewers has been positive. Also, the authors have been willing to perform the extra work required. The existence of the policy statement has helped since both the reviewers and the editors can refer to the policy statement and thus avoid rehashing the arguments with the authors. However, there were some particular difficulties.

1) The policy statement was phrased in such a way as to allow the editor to reject papers outright (without bothering reviewers) for failure to address the numerical accuracy issue. In practice, this seemed too severe and would have led to excessive publication lag since it would have put the numerical accuracy review/response in series with the other communications. Consequently, I often did initiate the review process even on papers that clearly did not abide by the policy. This also made it easier to be firm with the authors later, since I had the additional moral support of the reviewer's comments.

2) Some authors chose to abide by the letter of the law in the policy statement with generic statements that could be inserted into any paper, such as "the results from different grid resolutions were compared, and a 13×13 grid was shown to be adequate." Although our policy statement was not very demanding, I did reject such "trust me" statements and insisted on some quantifiable grid convergence results. As someone put it, "Convergence lies in the eyes of the beholder." I agree, but that is exactly the point of requiring some quantifiable criterion; it allows the reader to decide for himself. It would be naive in the extreme to think that there is any consensus agreement on what constitutes adequate convergence testing. We were not requiring a priori any particular method or any particular quantitative measure of convergence, but it is necessary to supply the reader with some *numbers.* Note that compliance with this requirement does not necessarily guarantee acceptance of the paper; it is still up to the reviewers and editors to exercise their own professional judgment on the adequacy of the quantified convergence criteria.

3) Some authors would prefer to refer to other papers on similar problems for the grid convergence test. This approach is legitimate in theory, and sometimes in practice, but for reasons noted in the previous paragraph, it is difficult and problematical. It is certainly preferable to have every paper self-contained in this regard.

Some of the papers submitted and accepted did *not* display very convincing convergence results. This again alludes to the difference of opinions mentioned previously, and it is a difficult subject. During my tenure as associate editor for *JFE,* I was quite liberal in accepting papers as long as the grid convergence numbers were provided so that the reader could judge for him- or herself. There are good and bad, sensitive, and insensitive indicators of convergence. As noted earlier, it is possible to be fooled by only looking at a neighboring problem. An obvious example is that of Poiseuille flow. If one tries to answer the question of "how many points are required to be in a boundary layer on an aerodynamics problem" by considering the neighboring problem of two-dimensional Poiseuille flow, one quickly comes to the conclusion that a single point in the boundary layer gives perfect accuracy! The obvious reason is that the solution to two-dimensional Poiseuille flow is a parabola, and therefore any second-order finite-difference method will give the exact answer.

Likewise, one can erroneously conclude that a uniform mesh is optimal.[10] A not-so-obvious bad indicator of grid convergence is the vortex wake solution. Many authors have "pointed with pride" to their quite accurate predictions (compared to experiment) of the Strouhal number for the near wake of a circular cylinder. It is apparently not very widely recognized that this is an easy calculation, because the frequency of the von Kármán vortex wake is essentially an inviscid phenomena, and therefore the accuracy of its prediction is not a good indicator of the accuracy of predicted boundary layer heat transfer, friction drag, or wake decay.

IV. Examples of What Can Be Done

I would like to point out a few exemplary publications addressing the question of the control of numerical accuracy. I have already mentioned the turbulence calculations of Shirazi and Truman,[3] Schonauer's ambitious approach,[5] and the work of Shih et al.[8] in which both the accuracy of the code (i.e., freedom from coding errors) and its second-order convergence for a particular problem are convincingly demonstrated. Another paper, by Kuruvila and Anderson,[11] is nicely illustrative of the difficulties and pitfalls of doing convergence studies with artificial dissipation terms in the equations. The paper by Fujii et al.[12] was illuminating in demonstrating the importance of grid resolution for Euler equation solutions to the leading edge separation problem. Thareja et al.[13] present solution-adaptive, nonstructured finite-element solutions of the supersonic blunt body problem, which include, in the methodology, the control of numerical accuracy. Dietrich et al.[14] present systematic grid truncation error testing of ocean circulation codes with four different methods. This procedure is so rare in the geophysical community as to be virtually nonexistent. The paper by Durst and Pereira[15] demonstrates that the entire procedure is readily applicable to time dependent problems as well as steady state problems. Blottner's paper[16] demonstrates his thorough tests for hypersonic nose tips. Nguyen and Maclaine-Cross[17] use Richardson extrapolation to zero mesh size to produce reliable curve fits to incremental pressure drop number in heat exchangers from full Navier-Stokes solutions. Finally, any such list, no matter how fragmentary, must include the classic study of the natural convection benchmark problem by de Vahl Davis.[18]

V. Conclusions and Recommendations

The control of numerical accuracy as addressed in the *Journal of Fluids Engineering* policy statement is a necessary but not sufficient component of the broader problem of code validation and verification. It is important to realize, however, that a code can be validated and verified and may be indeed certifiable as "error free," but this does not obviate the need for systematic grid convergence testing (or other systematic, quantitative error estimation) in any new application.

How far should we go? In research journals, I think a broad application of some numerical accuracy control philosophy would do much to improve the quality of published work. (Also, by putting a burden of more work on researchers, it would probably cut down on the number of papers. I, for one, would shed no tears.) In the long run, I would also be in favor of commercial certification of CFD codes. The American National Standards Institute and the American Society of Testing Materials are already involved in such certification activities in many areas, including FORTRAN compilers. I have some doubts, however, regarding the ability of such organizations to handle certification for complex CFD codes. It is probably worthwhile to consider now that AIAA and ASME may be active in the area of CFD code certification (and perhaps *de*certification) in the future. I hasten to add that this is *not* the kind of work that I would personally enjoy or am qualified to do. But, like it or not, I can envision seeing, in my lifetime, CFD code certification by professional societies or joint committees thereof. Note that CFD code certification was first suggested by Mehta.[19]

I do not particularly like the idea of CFD code certification, and perhaps many readers do not either. But *users* do, and if we do not involve ourselves, I think we will find ourselves frozen out. Clearly, users of CFD codes (not fellow CFD researchers, but real engineers interested in building something) want something that they can use with ease and confidence. Without a certification program, I am confident that simple "market forces" will not enforce high standards, but in fact will strongly favor pseudo-robust codes. By "pseudo-robust" I mean a code that appears to give a reasonable answer to most any problem. A truly robust code, which really does give a reasonably accurate answer to most any problem, is most difficult to achieve as we all know. From the user's point of view, certification is extremely important. In my own experience, it is a major consideration in codes for ground water hydrology studies. Older codes, with perhaps a 20-year history and correspondingly archaic FORTRAN styles, are inefficient, clumsy to use, unreadable, and therefore virtually unmodifiable; nevertheless, they are certified and they are the standards of performance for new codes.

Commercially available codes certified by some agency or professional society must include attempts to guard against misuse. It is of course impossible to fulfill this goal completely. In fact, the experience of many of our professional colleagues suggest that it is well nigh hopeless. (I asked a professional colleague at a national laboratory if his code was publically available, and he said no, but he would give it to me, because he knew or had a reasonable expectation that I would not misuse it.) CFD codes are much more difficult than linear algebra packages or statistical packages, but there are plenty of horror stories regarding the misuse of even these more straightforward codes. The reader may be of the opinion that we should not even turn loose on the world a general-purpose CFD code, but rather leave it in the hands of us "experts," at least until we can agree amongst ourselves. Unfortunately this agreement is not forthcoming, and in the meantime, commercial codes are already available (none of which is very impressive, in my opinion).

One thing that we (professionally) could require is that any code, in order to be certified, have built into it automatic error estimators, *not* as user options, but as hard-wired additional output. Like the experimental error bars on data, the error estimates can be ignored or incorporated by the practicing engineer according to his judgment, but he must be apprised of the estimates. There is a natural human desire for easy and unambiguous answers; it is our professional obligation to refuse to give them, in spite of "market forces," which I do not hold to be sacrosanct.

Appendix: Editorial Policy Statement on the Control of Numerical Accuracy†

A professional problem exists in the computational fluid dynamics community and also in the broader area of computational physics. Namely, there is a need for higher standards on the control of numerical accuracy.

The numerical fluid dynamics community is aware of this problem but, although individual researchers strive to control accuracy, the issue has not to our knowledge been addressed collectively and formally by any professional society or journal editorial board. The problem is certainly not unique to the *JFE* and came into even sharper focus at the 1980–81 AFOSR-HTTM-Stanford Conference on Complex Turbulent Flows. It was a conclusion of that conference's Evaluation Committee‡ that, in most of the submissions to the conference, it was impossible to evaluate and compare the accuracy of different turbulence models, since one could not distinguish physical modeling errors from numerical errors related to the algorithm and grid. This is especially the case for first order accurate methods and hybrid methods.

The practice of publishing comparisons based on coarse grid solutions, without systematic truncation error testing, may have been acceptable in the past. Certainly 10–15 years ago any calculation was of interest, and much of the exploratory work deserved publication, as many researchers lacked the computational power or funds to do a thorough and systematic error estimation. We are of the opinion that this practice, however understandable in the past, is outmoded and that, with powerful computers becoming more common, standards should be raised. Consequently, this journal hereby announces the following policy:

The Journal of Fluids Engineering will not accept for publication any paper reporting the numerical solution of a fluids engineering problem that fails to address the task of systematic truncation error testing and accuracy estimation.

Although the formal announcement of this journal policy is new, it has been the practice of many of our conscientious reviewers. Thus the present announcement is not a change in policy so much as a clarification and standardization.

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‡Emmons, H. W. (Chairman), "Evaluation Committee Report," pp. 979–986 in *Proc. 1980-81 AFOSR-HTTM-Stanford Conference on Complex Turbulent Flows,* Vol. II, "Taxonomies, Reporter's Summaries, Evaluation, and Conclusions," Thermosciences Division, Mechanical Engineering Department, Stanford University.

Methods are available to accomplish this task, such as Richardson extrapolation (when applicable), calculations with a high- and low-order method on the same grid, and straightforward repeat calculations with finer or coarser grids. As in the case of experimental uncertainty analysis, "...any appropriate analysis is far better than none as long as the procedure is explained."§ Whatever the authors use will be considered in the review process, but we must make it clear that *a single calculation in a fixed grid will not be acceptable,* since it is impossible to infer an accuracy estimate from such a calculation. Also, the editors will not consider a reasonable agreement with experimental data to be sufficient proof of accuracy, especially if any adjustable parameters are involved, as in turbulence modeling.

We recognize that it can be costly to do a thorough study, and that many practical engineering calculations will continue to be performed on a single fixed grid. However, this practice is insufficient for publication in an archival journal.

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