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SPECIAL NOTE

A NOTE ON NUMERICAL ACCURACY

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INTRODUCTION

This note is concerned with evaluation of the accuracy of numerical solutions of partial differential equations (PDEs), especially in fluid mechanics. Most of the ideas are not original but they appear to be under-appreciated and under-utilized at present.

Knowledge of the accuracy of a method is essential to any user. Unfortunately, many published papers do not provide error estimates. In others, the method of comparison does not provide the information potential users would like to have.

Fluid flows of engineering interest are very difficult to calculate. Nearly all are turbulent flows. They often contain such additional complications as chemical reaction, two phases, non-Newtonian behavior, and complex geometry. Except in very simple flows, these effects are represented by models whose accuracy needs to be assessed. To do so requires that other error sources (including numerical ones) must be eliminated or, at least, be accurately known.

TYPES OF NUMERICAL ERRORS

For simplicity, we consider only steady flows and assume that the problem (equations plus boundary conditions) has a unique, exact solution. Of course, some problems have multiple steady solutions. However, if the solutions are well-separated, an initial guess sufficiently close to one solution should allow the method to converge to that solution.

Any numerical method should be convergent in the mathematical sense that it produces the exact solution of the PDEs as the grid size (or equivalent parameter) vanishes. The rate at which the error, defined as the difference between the numerical and exact solutions, is reduced, as the grid is refined, is an important property of a method.

It is common for authors to test methods by comparing their solutions with ones obtained by other methods. This is not an optimum test and can even be misleading. The differences between the various solutions are often simply differences in errors; consequently, it is difficult to evaluate which is the better method. Comparison with the exact solution of the PDEs (i.e. accurate error estimation) is a more significant measure of quality. The best test of a numerical method is whether it gives the exact solution at lower cost than its competitors; it is also worthwhile to remember that a single method may not be the best for all problems.

Comparisons with experimental data require care, especially when modeling approximations are employed. Laboratory data contain errors which need to be evaluated and the data should not fit more closely than the experimental uncertainty. So, for assessing the accuracy of a numerical method, comparison with the exact solution of the problem (which includes any errors due to model inaccuracy) is a better test than comparison with experiments.

ESTIMATION OF NUMERICAL ERRORS

Errors arise from the various components of a numerical method: iteration procedure, grid generation (including co-ordinate transformations), and discretization (finite difference, volume, or element).

Some methods require many iterations to converge. In most codes, iteration is stopped when the difference between two successive iterates is less than some preselected level. Unfortunately, the convergence error, defined as the difference between the current iterate and the exact solution of the discretized equations depends not only on the difference between successive iterates but also on the rate of convergence. It is possible to estimate the convergence error; this estimate provides a better basis for a stopping criterion.

As noted above, grid generation and discretization errors are the difference between the converged solution and the exact solution of the PDEs. The latter may be obtained using very fine grids; such benchmark solutions exist in the literature for selected problems.

An alternative method of error estimation is Richardson's method. It is based on expressing the error as a Taylor series in some parameter, h, that can be regarded as the grid size, computing the solution on at least two different grids and calculating the error from the differences. The cost is relatively small. In two-dimensions, a coarse grid calculation costs approximately one-tenth that of the fine grid calculation. With grid refinement methods, the coarse grid solution costs nothing. The error estimates are accurate only for small h. However, for large h, the error estimates, although inaccurate, are large and indicate that the solution is inaccurate, thus serving the intended purpose.

CONCLUSION

Knowledge of the accuracy of any procedure is essential to successful use of that method. This is especially true of numerical methods for solving PDEs. Authors should therefore provide information that potential users need to evaluate the accuracy of the method; this will help potential users to evaluate the method and increase the chances of its adoption. Both estimation of the accuracy of the new method and comparisons with the accuracy of existing methods should be routine elements of any presentation of a new method. Finally, it is hoped that this note will stimulate much needed discussion of the issues raised.

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