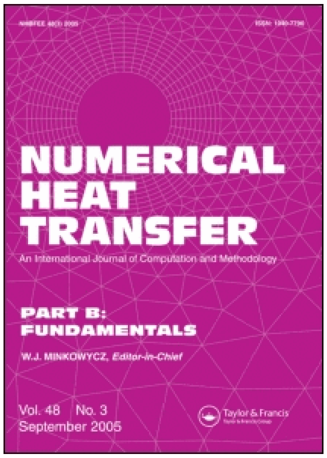

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ESTIMATE OF ITERATION ERRORS IN COMPUTATIONAL FLUID DYNAMICS

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In this work an empirical estimator is used to estimate the iteration error based on the convergence rate of the variable of interest. Problems of heat transfer and of fluid mechanics are solved by the finite-difference and finite-volume methods using various iteration methods. In the initial iterations the accuracy of the empirical estimator is usually low; when the number of iterations is high, round-off errors predominate over iteration errors, but even so, the accuracy is relatively good; and in the interval between these two extremes, the accuracy tends to improve as the number of iterations increases.

INTRODUCTION

According to [1–6], numerical errors are caused by a variety of sources: truncation errors (E_T), round-off errors (E_π), programming errors (E_p), and iteration errors (E_n). Symbolically, one has

$$E(\phi) = E(E_T,\ E_\pi,\ E_p,\ E_n) \tag{1}$$

where ϕ is the variable of interest, which may be local or global, primary or secondary. These four sources of error can have different magnitudes and signs, which may result in partial or total cancellations between these errors. The definition, effect, and origin of each of these four sources of error are discussed in [7].

The literature [1, 3, 6, 8, 9] reports several criteria for interrupting iterative processes. Two very common ones [9] are based on (1) the difference of the variable between two successive iterations and (2) the residue of the discretized equations.

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NOMENCLATURE

E	numerical or iteration error
L	length of the problem domain, m
n	iteration
N	number of nodes
p	pressure, Pa
p_L	asymptotic order of the iteration error
p_U	apparent order of the iteration error
u	component of the velocity vector in the x direction, m/s
U	uncertainty or estimate of the numerical or iteration error
v	component of the velocity vector in the y direction, m/s
x	Cartesian spatial coordinate in the horizontal direction, m
y	Cartesian spatial coordinate in the vertical direction, m
Λ	dependent variable
θ	effectiveness
μ	mass flow rate, kg/s
ϕ	numerical solution of the variable of interest
Φ	exact analytical solution of the variable of interest
ψ	convergence rate

Subscripts

n	iteration
1	iteration $n-2$
2	iteration $n-1$
3	iteration n
∞	estimate of the exact solution

However, they do not estimate the true iteration error. With these criteria, an iterative process can be interrupted very prematurely [8] or very belatedly in relation to the value of the desired error.

Two procedures to estimate the true iteration error effectively are given in [1, 8]. However, Ferziger and Peric [1] apply their estimator only to norms of field-dependent variables, while Roy and Blottner [8] apply their estimator to a local variable but do not compare the estimated error and the true error.

The purpose of the present work is to test an iteration error estimator on the local and global variables of three heat transfer and fluid mechanics problems. The error estimates are compared with the true error. With this work, we intend to expand the application and understanding of type [1] estimators.

The importance of a reliable and accurate iteration error lies in interrupting the iterative process when one reaches the desired level of error for the variable of interest. This saves CPU time because the iterative process is not interrupted belatedly. In addition, by interrupting the iterative process prematurely, one avoids having a high level of iteration error that affects the numerical error and the modeling error.

In the following sections, the iteration error is characterized and a procedure is presented to estimate the iteration error using an *empirical estimator*. Examples of application are given involving one-dimensional and two-dimensional heat diffusion in a steady-state and two-dimensional isothermal flow of incompressible fluid. The numerical solutions to these problems are obtained by the finite-difference and finite-volume methods. The article ends with our conclusion about this work.

ITERATION ERROR

References [1, 3, 6, 8, 9] are examples of studies that discuss iteration errors. According to [1], considering a given variable of interest (ϕ), the iteration error (E) is the difference between the exact solution (Φ) of the discretized equations and the numerical solution in a given iteration (ϕ_n); in other words,

$$E(\phi_n) = \Phi - \phi_n \tag{2}$$

where the discretized equations result in the application of a numerical method on a mathematical model; and n represents the number of the current iteration in the process of solution of the system of algebraic equations obtained from the discretized equations of the mathematical model.

Among others, some factors that generate iteration errors are

1. The use of iterative methods to solve the system of algebraic equations
2. The use of segregated methods to obtain the solution for mathematical models constituted of more than one differential equation
3. The existence of nonlinearities in the mathematical model

The principal characteristic of iteration errors involved in iterative processes that present a monotonic convergence rate is that, when one increases the number of iterations, their value generally decreases on a logarithmic scale and tends toward a constant inclination. This is illustrated in Figure 1, which shows the iteration error resulting from the solution of a quadratic equation ($x^2 - 5x + 6 = 0$) by the fixed-point iteration method [10], with an initial condition of $x_0 = 0$. Hence,

$$E(\phi_n) = C10^{-np_L} \tag{3}$$

where C is a constant and p_L is the asymptotic order representing the inclination toward which the curve of the error tends when $n \to \infty$. The greater this inclination in relation to the axis of the abscissas (Figure 1), the greater is the reduction rate of the iteration error (E) with the increase of n. Moreover, for the same number of iterations, the error is smaller.

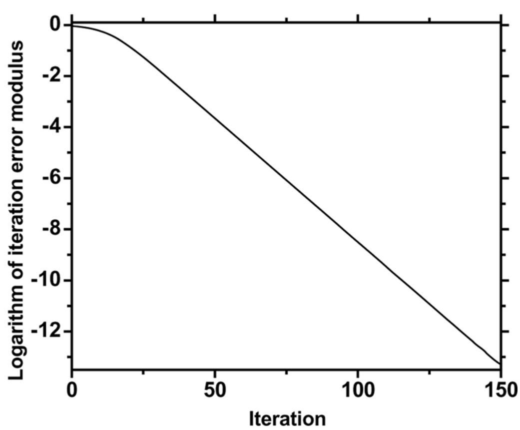

Figure 1. Behavior presented by iteration errors.

The value of the iteration error can only be calculated with Eq. (2) when one knows the exact solution of the system of equations resulting from the discretization of the mathematical model. But this is not usually the case in practical terms. Therefore, it is necessary to estimate the value of the exact solution. To this end, a procedure is presented in the next section.

AN EMPIRICAL ESTIMATOR

The uncertainty (U) of the numerical solution for a variable of interest (ϕ) is calculated by the difference between the estimate of the exact solution (ϕ_∞) of the system of equations and its numerical solution in an n iteration (ϕ_n), that is,

$$U(\phi_n) = \phi_\infty - \phi_n \tag{4}$$

where the uncertainty is also called estimated iteration error. By analogy to Eq. (3), one admits that

$$U(\phi_n) = k10^{-np_U} \tag{5}$$

where k is a constant and p_U is the apparent order of the uncertainty. The exponent p_U represents the local inclination of the uncertainty curve (U) versus the number of iterations (n) on a graph such as the one shown in Figure 1. Considering the iterations n_1, n_2, and n_3, with $n_1 < n_2 < n_3$, and Eqs. (4) and (5), one has

$$\begin{cases} \phi_\infty - \phi_{n_1} = k10^{-n_1 p_U} \\ \phi_\infty - \phi_{n_2} = k10^{-n_2 p_U} \\ \phi_\infty - \phi_{n_3} = k10^{-n_3 p_U} \end{cases} \tag{6}$$

In the system of Eq. (6), the unknows are ϕ_∞, k, and p_U. Solving it for ϕ_∞, one has

$$\phi_\infty = \phi_{n_3} + \frac{(\phi_{n_3} - \phi_{n_2})}{(\psi - 1)} \tag{7}$$

where

$$\psi = \frac{\phi_{n_2} - \phi_{n_1}}{\phi_{n_3} - \phi_{n_2}} \tag{8}$$

and the expression for the apparent order (p_U) can be seen in [11]. Substituting this result in Eq. (4), one reaches

$$U(\phi_{n_3}) = \frac{(\phi_{n_3} - \phi_{n_2})}{(\psi - 1)} \tag{9}$$

which constitutes an empirical estimator for iteration errors.

In [12] it is demonstrated that estimates of error based on equations similar to Eq. (9) are valid only for $\psi > 1$ or $\psi < -1$. Reference [11] demonstrates that the estimators of [1] and [8] are equivalent to the empirical estimator of the present work.

Criteria for Measuring the Performance of an Error Estimate

The quality of an error estimate can be evaluated by its effectiveness (θ), which is defined by the ratio of its uncertainty (U) and error (E) [13], that is,

$$\theta = \frac{U}{E} \tag{10}$$

An ideal error estimate is one whose effectiveness is equal to the unit ($\theta = 1$), that is, when the uncertainty is equal to the error ($U = E$). When the magnitude of the uncertainty is greater than the magnitude of the iteration error and both have the same sign, one can state that the error estimate is reliable [7], that is,

$$\theta \geq 1 \tag{11}$$

If the magnitude of the uncertainty is approximately equal to that of the iteration error, the error estimate is called accurate [14], that is,

$$\theta \approx 1 \tag{12}$$

The quantitative definition of what an accurate error estimate is depends on how close to the unit the effectiveness should be, which is a function of each case.

RESULTS

This section describes and presents numerical results for three problems, which are used to illustrate the application of the empirical estimator to iteration errors through examples of calculation. Many other results can be seen in [11].

One-Dimensional Poisson Equation

Problem 1 consists of one-dimensional heat diffusion, in a steady state, with heat absorption [15], which results in Poisson's equation, given by

$$\frac{d^2\Lambda}{dx^2} = 12x^2 \tag{13}$$

with Dirichlet-type boundary conditions on the two boundaries: $\Lambda(0) = 0$ and $\Lambda(L) = 1$; with $L = 1$. The numerical model is constituted of the finite-difference method [4], with second-order numerical approximations by means of a central difference and a uniform grid.

In this problem, four variables of interest (ϕ) were defined, namely, the numerical results at three specific nodes of the grid, that is, $\Lambda(L/2), \Lambda(9L/10)$ and $\Lambda(L/5)$, and the arithmetic mean of the numerical results obtained at all the nodes of the grid. Each variable of interest was subjected to an analysis of its iteration error (E), the estimate of the iteration error (U), the convergence rate (ψ), the apparent order (p_U), and the effectiveness (θ).

Table 1. Numerical results for $\Lambda(L/2)$, Problem 1

Grid (nodes)	n (iterations)	ϕ_n	$E(\phi_n)$	$\frac{U(\phi_n)}{E(\phi_n)}$
11	150	6.49999E−02	8.17368E−08	9.99999E−01
101	15,933	6.25249E−02	2.78104E−08	1.00030E+00
201	63,688	6.25062E−02	2.72793E−08	9.97596E−01

Numerical solutions were obtained for grids with $N = 11, 101,$ and 201 nodes. The system of equations resulting from the discretization of the mathematical model was solved with the Gauss-Seidel iteration method [10], using three types of initial conditions: null, unitary, and linear with x. A minimum drop of five orders of magnitude in the iteration error for all the variables of interest was considered the convergence criterion for the iterative process.

Table 1 presents the results for $\Lambda(L/2)$, as a function of the number of nodes of the grid, for the null condition, in the iteration in which the convergence criterion is met. As can be seen in this table, the error estimates show a high accuracy ($\theta \approx 1$). Analogous behavior was obtained for the other variables of interest, in every case. With the variation of the initial conditions described earlier, and the number of nodes of the grid, nine cases were considered and are described in Table 2. This table shows that the convergence rate (ψ) and the apparent order (p_U) vary only with the number of nodes in the grid. Therefore, they are not altered by changes in the initial conditions or the variable of interest.

The results of Problem 1 revealed two types of behavior. In the initial iterations, the error estimates are generally inaccurate and unreliable. After these initial iterations, however, the estimates become increasingly accurate. As can be seen in Figure 2, for example, there is discordance between uncertainty and error only in the initial iterations. It was found that, in these iterations, the convergence rate presents values lower than one ($\psi < 1$), which renders the application of the empirical estimator inadequate, according to [12].

Two-Dimensional Laplace Equation

Problem 2 consists of two-dimensional heat diffusion, in a steady state, without heat generation and with constant thermal conductivity [15], which results in Laplace's equation, given by

$$\frac{\partial^2 \Lambda}{\partial x^2} + \frac{\partial^2 \Lambda}{\partial y^2} = 0 \tag{14}$$

Table 2. Convergence rate (ψ) and apparent order (p_U) for Problem 1

Grid (nodes)	Cases	ψ	p_U
11	1, 2, 3	1.10557	0.04358
101	4, 5, 6	1.00098	0.00042
201	7, 8, 9	1.00024	0.00010

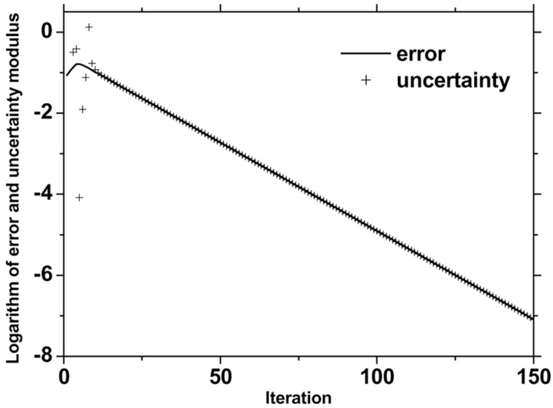

Figure 2. Error (E) and uncertainty (U) for $\Lambda(L/2)$, Problem 1, grid with 11 nodes.

with Dirichlet boundary conditions given by $\Lambda(0,y) = \Lambda(x,0) = 0$, $\Lambda(L,y) = y$, $\Lambda(x,L) = x$; and a square domain of unitary sides $(L = 1)$. The numerical model consists of the finite-difference method [4], with second-order numerical approximations through a central difference and uniform grids. In this case there is no discretization error [16], which facilitates the analysis of the iteration errors. In this problem, the variables of interest are the temperature at the center of the domain, that is, $\Lambda(L/2, L/2)$; and the mean temperature in the domain (Λ_m).

The numerical solutions were obtained for three different grids, as indicated in Table 3. The system of equations resulting from the discretization of the mathematical model was solved by the Gauss-Seidel iteration method. A multigrid method for linear problems was also used, whose algorithm is described on pages 169 and 170 of [4]. The null condition was used in all the cases. The convergence criterion adopted was a minimum drop of seven orders of magnitude in the iteration error for the two variables of interest.

Table 3 presents some numerical solutions for Problem 2, Eq. (14), calculated for the temperature in the center of the domain, whose exact solution is $\Phi = 1/4$, in the iteration in which the convergence criterion is satisfied in each case. Without the use of the multigrid, a behavior similar to that presented in Problem 1 occurred, that is, discordance between uncertainty and error only in the initial iterations, as shown in Figure 3. This figure also shows the behavior presented by other iteration error

Table 3. Numerical results for $\Lambda(L/2, L/2)$, Problem 2

Grid (nodes)	Method	n (iterations)	ϕ_n	$E(\phi_n)$	$\frac{U(\phi_n)}{E(\phi_n)}$
17 × 17	Without multigrid	397	2.49999E−01	9.80008E−08	1.00000E+00
33 × 33	Without multigrid	1,596	2.49999E−01	9.92262E−08	1.00002E+00
65 × 65	Without multigrid	6,331	2.49999E−01	9.98782E−08	1.00135E+00
17 × 17	With multigrid	22	2.50000E−01	−5.34994E−08	1.71884E+00
33 × 33	With multigrid	29	2.50000E−01	−7.68770E−08	2.77543E+00
65 × 65	With multigrid	35	2.49999E−01	2.70002E−08	1.54320E+01

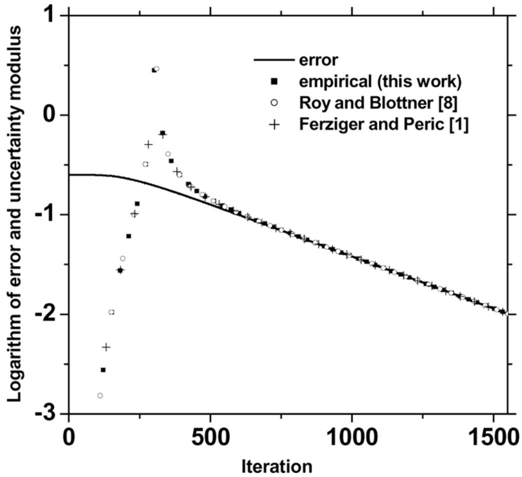

Figure 3. Error (E) and uncertainty (U) for $\Lambda(L/2, L/2)$, Problem 2, grid of 65×65 nodes, without multigrid.

estimators available in the literature, Ferziger and Peric's [1] and Roy and Blottner's [8] estimators. All the estimators presented similar results. After these initial iterations, the estimates become increasingly accurate.

With the use of the multigrid method, it was found that the iteration error does not present monotonic behavior. As a result, the empirical estimator becomes inefficient in any iteration, presenting low accuracy and proving unreliable. This is illustrated in Figure 4, which also shows the behavior presented by the other estimators. All are inadequate when the multigrid method is used.

Note, in Table 4, that the convergence rate (ψ) and the apparent order (p_U) vary with the number of nodes in the grid. For a finer grid (65×65) there is a slight

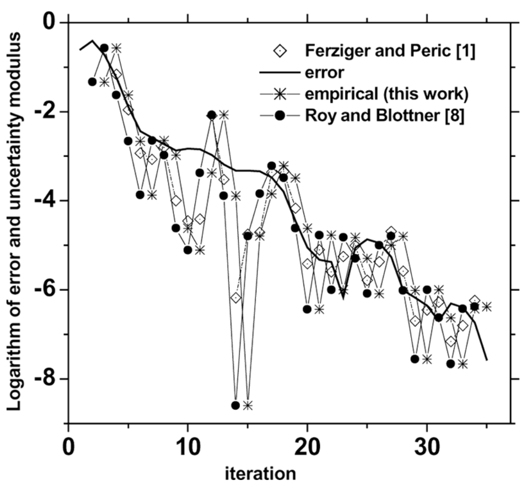

Figure 4. Error (E) and uncertainty (U) for $\Lambda(L/2, L/2)$, Problem 2, grid of 65×65 nodes, with multigrid.

Table 4 Convergence rate (ψ) and apparent order (p_U) for Problem 2

Grid (nodes)	Variable	ψ	p_U
17×17	$\Lambda(1/2, 1/2)$	1.03956	0.01685
17×17	Λ_m	1.03956	0.01685
33×33	$\Lambda(1/2, 1/2)$	1.00970	0.00419
33×33	Λ_m	1.00970	0.00419
65×65	$\Lambda(1/2, 1/2)$	1.00241	0.00104
65×65	Λ_m	1.00238	0.00103

difference between the convergence rate of $\Lambda(L/2, L/2)$ and Λ_m, probably due to the effect of the round-off errors, although, according to [3], different variables involved in the same iterative process may present different convergence rates.

Two-Dimensional Navier-Stokes Equations

The mathematical model of the Problem 3 consists of the conservation of mass law and the conservation of momentum law (Navier-Stokes equations). The simplifications considered for the problem are steady state; two-dimensional flow in the x and y directions; incompressible fluid; density and viscosity of the fluid are constant; and without other effects.

Problem 3 consists of the two-dimensional flow inside a square cavity, with unitary sides, whose lid moves. A source term is added in order to obtain an analytical solution [17] for the three unknowns: two velocity components (u, v) and the pressure (p).

The numerical solution for this problem is obtained by the finite-volume method [1] with second-order numerical approximations through a central difference, uniform grid, and co-located arrangement of variables. The MSI iteration method [18] was used to solve the systems of equations resulting from the discretization of the mathematical model. In this case there is discretization error. Therefore, analytical solutions are not considered to analyze the iteration errors. So, one considers the "exact" iteration solution at the limit of "machine error," that is, the numerical solution obtained along the iterative process when there are no more iteration errors and only round-off errors remain.

To analyze the performance of the empirical estimator, four variables of interest were considered: the numerical results of u, v, and p at the center of the domain, that is, $u(1/2, 1/2), v(1/2, 1/2)$, $p(1/2, 1/2)$; and the mass flow circulating in the

Table 5. Numerical results for $u(1/2, 1/2)$ and $p(1/2, 1/2)$, Problem 3

Variable	Grid (nodes)	n (iterations)	ϕ_n	$E(\phi_n)$	$\frac{U(\phi_n)}{E(\phi_n)}$
u	16×16	728	–2.43644E–01	–9.36800E–11	1.00418E+00
u	32×32	1,171	–2.48363E–01	–1.11803E–09	1.00027E+00
u	64×64	2,160	–2.49587E–01	–2.18090E–10	1.04103E+00
p	16×16	728	1.54559E+00	–7.18439E–10	1.01397E+00
p	32×32	1,171	1.54543E+00	2.13074E–09	1.02625E+00
p	64×64	2,160	1.54533E+00	1.08271E–09	1.09693E+00

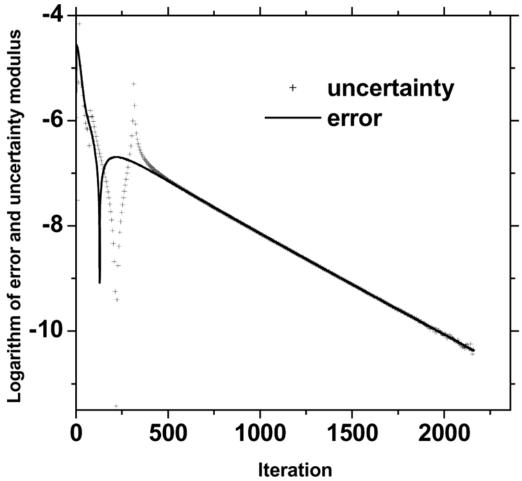

Figure 5. Error (E) and uncertainty (U) for μ, Problem 3, 64 × 64 grid.

cavity (μ). The numerical solutions were obtained for grids with 16 × 16, 32 × 32 and 64 × 64 control volumes. Analogously to Problems 1 and 2, the iteration error (E), the estimate of the iteration error (U), the convergence rate (ψ), the apparent order (p_U), and the effectiveness (θ) were analyzed for all the grids and each variable of interest. Table 5 presents the number of iterations (n) that were required to satisfy the convergence criterion adopted: minimum drop of seven orders of magnitude in the nondimensionalized residue (R^*) of the discretized equations [9].

In Table 5, note that in all the grids considered for the variables $u(1/2, 1/2)$ and $p(1/2, 1/2)$, the empirical estimator presented reliable, that is, $\theta > 1$, and accurate results at the end of the iterative process. Figure 5 illustrates the behavior obtained for the numerical error and for the uncertainty of the mass flow circulating in the cavity (μ) and grid of 64 × 64 control volumes. The behavior is similar for the other variables and cases. Note, in Table 6, that the convergence

Table 6. Convergence rate (ψ) and apparent order (p_U) for Problem 3

Grid (nodes)	Variable	ψ	p_U
16 × 16	$u(1/2, 1/2)$	1.03612E+00	1.54100E−02
16 × 16	$v(1/2, 1/2)$	1.01655E+00	7.13009E−03
16 × 16	$p(1/2, 1/2)$	1.01580E+00	6.80914E−03
16 × 16	μ	1.01439E+00	6.20720E−03
32 × 32	$u(1/2, 1/2)$	1.00881E+00	3.81185E−03
32 × 32	$v(1/2, 1/2)$	1.00948E+00	4.09874E−03
32 × 32	$p(1/2, 1/2)$	1.00928E+00	4.01360E−03
32 × 32	μ	1.00881E+00	3.81259E−03
64 × 64	$u(1/2, 1/2)$	1.00459E+00	1.98928E−03
64 × 64	$v(1/2, 1/2)$	1.00505E+00	2.18967E−03
64 × 64	$p(1/2, 1/2)$	1.00446E+00	1.93694E−03
64 × 64	μ	1.00460E+00	1.99342E−03

rate (ψ) and the apparent order (p_U) for this problem vary with the number of volumes of the grid, which also holds true for Problems 1 and 2.

CONCLUSION

An empirical estimator was analyzed to estimate iteration errors in numerical simulations. The iteration error was defined as the difference between the exact numerical solution of the system of equations and the numerical solution in a given iteration. This estimator provides an estimate of the iteration error based on the convergence rate of the variable of interest, according to the theory presented herein.

Based on the uncertainty and error ratio, the behavior of the empirical estimator was analyzed with respect to its accuracy and reliability. In the tests with Poisson's equation, Problem 1, two types of behavior were observed. In the initial iterations, a maximum of 13% of the total number of iterations, the error estimates (uncertainties) are inaccurate and unreliable. After these initial iterations, the estimates are increasingly accurate.

In the test involving the Laplace equation, Problem 2, without using the multigrid method, similar behavior was found to that obtained in Problem 1, that is, discordance between uncertainty and error occurs only in the initial iterations. However, in these tests, the initial iterations correspond, at most, to 9% of the total number of iterations. For the tests involving the application of the multigrid method, the empirical estimator did not prove efficient since it presented low accuracy and fairly unreliable results.

An analysis of the behavior of the iteration error involved in the numerical solution of the Navier-Stokes equations, Problem 3, found that the iteration error itself presented oscillations in the initial iterations, as well as uncertainty. This had not occurred in the two previous problems. As for the efficiency of the error estimator, results similar to those of Problems 1 and 2 were obtained, although in Problem 3, the initial iterations correspond at the most to 17% of the total number of iterations involved in the calculation.

Overall, in the numerical tests performed here, the performance of the empirical estimator can be divided into three intervals: (1) in the initial iterations, the accuracy is generally low; (2) when the number of iterations is very high, the round-off errors affect the accuracy, which is nonetheless good; and (3) in the interval between these two extremes, the accuracy tends to be great as the number of iterations increases.

The empirical estimator is not recommended for use in iterative processes that employ the multigrid method, because the iteration error does not exhibit monotonic behavior. However, due to their wide application in computational fluid dynamics (CFD), it is important to improve the performance of iteration error estimators in problems solved with the multigrid method. The present authors are working toward this objective, as well as expanding the tests of the empirical estimator on problems of compressible and reactive fluid and on natural and forced convection.

Equivalence was found to exist between the empirical estimator and other iteration error estimators available in the literature, Ferziger and Peric's [1] and Roy and Blottner's [8] estimators. The estimator of [1] and that of this work provide a more accurate and reliable estimate of the iteration error than do the criteria based on the difference of the variable between two successive iterations or in the residue of the discretized equations. Nonetheless, it appears that the estimators must be applied to local and global variables and not to norms of field variables.

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